

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 2000

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

Telephone +420 2 20390 111
Telefax +420 2 2092 0661
E-mail postmaster@icpf.cas.cz
Internet <http://www.icpf.cas.cz>

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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 functions as a center for fundamental research in chemical, biochemical, catalytic and environmental engineering. Besides these activities, the Institute acts as a graduate school for PhD studies in the field of chemical engineering, physical chemistry, industrial chemistry, and biotechnology.

MANAGEMENT

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

DEPARTMENTS

Department of Diffusion and Separation Processes	(page 5)
E. Hála Laboratory of Thermodynamics	(page 11)
Department of Catalysis and Reaction Engineering	(page 17)
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STAFF
(31 December 2000)

Category	Number of Employees
Research	109
Technical	26
Administrative	16
Services	12

BUDGET 2000
(in million Kč; 39 Kč = 1 US\$, approx.)

Institutional support from National Budget	51
Research funds from Grant Agencies	34
Contracts with industry	1

Abbreviations used throughout the Report

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

Department of Diffusion and Separation Processes

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

Fields of research

- Transport during vapor permeation and pervaporation processes; the effect of sorption of permeating molecules on the diffusion coefficient
- Relation between the morphology and application properties of polymer catalysts and adsorbents
- Hydrodynamic study of two-phase counter-current gas-liquid flow in column with packed and bubble bed in series
- Amine extraction of sulfuric acids; liquid-liquid extraction of heavy metals; determination of organic pollutants in water
- Liquid extraction of drinking and surface waters for determination of toxic pollutants
- Supercritical fluid extraction of essential oils; enzymatic reactions in supercritical CO₂; solubilities of liquids and solids in dense CO₂ with entrainer

Applied research

- Extraction aided determination of organic pollutants in waters
- Extraction refining of digitalis plant alkaloids (was put into operation)
- Refining of plant extracts
- Preparation of corundum support for ceramic membranes
- Analysis of function of the catalytic reactor for bisphenol A synthesis and research of the catalytic deactivation

Research projects

Hypersulfonated ion exchanger catalysts

(K. Jeřábek, supported by GA CR, grant No. 104/99/0125)

The possibilities are examined of an increase of catalytic activity of ion exchanger resin catalyst by increasing the degree of their sulfonation beyond the conventional limit of one sulfonic group per monomer unit. It has been found that for proper assessment of the

hypersulfonated resin catalysts it is necessary to consider both the influence of the hypersulfonation on the quality of the active centers and the changes in the resin backbone morphology. [Refs. 19-23]

Molecular accessibility of microporous matrixes

(K. Jeřábek, joint project with the University of Padua, Italy; co-operation project CNR/ASCR)

Metal catalysts supported on polymer carriers were investigated, especially as to the accessibility of metal nanoparticles inside the gel polymer matrix. [Refs. 1, 2]

Study of deactivation of ion exchanger catalysts for synthesis of bisphenol A

(K. Jeřábek, supported by GA ASCR, grant No. S4072002)

Analysis of the behaviour of the industrial reactor for bisphenol A synthesis and laboratory modelling of the catalyst ageing are used for elucidation of the origin of the catalyst deactivation.

Catalysis inside macromolecular matrixes

(K. Jeřábek, co-operation with the Universities of Padua and L'Aquila, Italy; project No. 27/60, Agreement on scientific and technical co-operation between Italy and Czech Republic)

Specific properties of polymers useful as catalyst supports were investigated using combined experimental techniques like inverse steric exclusion chromatography, EPR and NMR. [Ref. 8]

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

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

The pressure and liquid hold up overshoot following sudden increase of gas or liquid flow have been measured in counter-current packed bed column. The results have been described by a mathematical model. Experimental study of hydrodynamic behaviour of two-phase counter-current gas-liquid flow in column with packed and bubble bed in series has been evaluated. [Refs. 9, 12, 25, 26, 30-32]

Extraction of molybdenum and tungsten by tertiary amines

(A. Heyberger, supported by GA CR, grant No. 104/98/1440)

Results of measurements of sulfuric acid extraction from aqueous solutions with trialkylamine in octanol/kerosene mixtures were correlated. Extraction of tungsten from aqueous solutions of sodium tungstate with solutions of trialkylamine in mixtures of tributyl phosphate in kerosene was investigated. Before the extraction, the organic phase was presaturated with sulfuric acid. Measurements at various values of constant pH were compared. [Refs. 6, 10, 16, 27]

Continuous liquid extraction of drinking and surface waters for determination of toxic and ultratrace pollutants

(A. Heyberger, supported by GA CR, grant No. 104/99/1469)

New equipment VPE for determination of organic pollutants was patented. [Ref. 14]

Solubilities in supercritical fluids - measurement and modelling

(H. Sovová, supported by GA CR, grant No. 203/98/1445)

Optimal conditions for the extraction of essential oils from seeds containing vegetable oils were determined. The solubility increase of β -carotene and ferulic acid in supercritical CO₂ with ethanol as entrainer was measured. [Ref. 28, 29]

New way of preparing γ - and α -linolenic fatty acids from *Ribes nigrum* seeds: Enzymatic catalysis in supercritical carbon dioxide

(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry and ICT, supported by GA CR, grant No. 203/99/1457)

Hydrolysis of black currant oil dissolved in supercritical CO₂ was studied using a continuous reactor. The reaction was catalyzed by immobilised lipase Lipozyme. Further, literature on enzymatic reactions in supercritical fluids was reviewed. Solubility of oils from black currant seed and from grape seed in supercritical carbon dioxide was measured and relation between the oil composition and its solubility in CO₂ was derived. [Ref. 11]

International co-operations

Otto von Guericke University of Magdeburg, Germany: Determination of porous structure of ceramic membranes

Hiroshima University, Japan: Pervaporation on ceramic membranes

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

Technical University, Bratislava, Slovakia: Polymer supported catalysts

University of Strathclyde, Glasgow, Great Britain: Morphology of functional polymers

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

Institute of Chemical Engineering, Sofia, Bulgaria: Separation of heavy metals from aqueous solutions using amine extractants; high-pressure phase equilibria

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

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

Visits abroad

A. Heyberger: University of Durban, AECI, CSIR, Johannesburg, Republic of South Africa

K. Jeřábek: University of Padua, Italy

P. Uchytíl: Otto von Guericke University of Magdeburg, Germany

Visitors

I. Mishonov, Institute of Chemical Engineering, Sofia, Bulgaria

R. Tomovska, University of Skopje, Macedonia

B. Hutton, CSIR, Johannesburg, Republic of South Africa

P. Myburgh, CSIR, Johannesburg, Republic of South Africa

Teaching

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

Publications

Papers

1. Biffis A., Landes H., Jeřábek K., Corain B.: Metal palladium dispersed inside macroporous ion-exchange resins: the issue of the accessibility to gaseous reactants. *J. Mol. Catal. A: Chem.* 151, 283-288 (2000).
2. D'Archivio A. A., Galantini L., Biffis A., Jeřábek K., Corain B.: Polybenzimidazole as a promising support for metal catalysis: morphology and molecular accessibility in the dry and swollen state. *Chem. Eur. J.* 6(5), 794-799 (2000).
3. Howdle S. M., Jeřábek K., Leocorbo V., Marr P. C., Sherrington D. C.: Reversibly collapsible macroporous poly(styrene-divinylbenzene) resins. *Polymer* 41 (19), 7273-7277 (2000).
4. Jiříčný V., Siu S., Roy A., Evans J. W.: Regeneration of zinc particles for zinc-air fuel cells in a spouted-bed electrode. *J. Appl. Electrochem.* 30, 647-656 (2000).
5. Jiříčný V., Roy A., Evans J. W.: Electrodeposition of zinc from sodium zincate/hydroxide electrolytes in a spouted bed electrode. *Metall. Mater. Trans.* 31B(4), 755-766 (2000).
6. Poposka F., Procházka J., Tomovska R., Nikolovski K., Grizo A.: Extraction of tartaric acid from aqueous solutions with tri-iso-octylamine (HOSTAREX A 324). Equilibrium and kinetics. *Chem. Eng. Sci.* 55(9), 1591-1604 (2000).
7. Uchytíl P., Schramm O., Seidel-Morgenstern A.: Influence of the transport direction on gas permeation in two-layer ceramic membranes. *J. Membr. Sci.* 170, 215-224 (2000).
8. Biffis A., D'Archivio A. A., Jeřábek K., Schmid G., Corain B.: The generation of size-controlled palladium nanoclusters inside gel-type functional resins: arguments and preliminary results. *Adv. Mater.* 12(24), 1909-1912 (2000).
9. Jiříčný V., Staněk V., Svoboda P., Ondráček J.: Experimental study of the flooding and appearance of a bubble-bed on top of a counter-current packed bed column. *Ind. Eng. Chem. Res.* (in press).
10. 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* (in press).
11. Sovová H.: Solubility of two vegetable oils in supercritical CO₂. *J. Supercrit. Fluids* (in press).
12. Staněk V., Svoboda P., Jiříčný V.: Experimental observation of pressure and holdup overshoot following a sudden increase of liquid flow. *Ind. Eng. Chem. Res.* (in press).

Review papers

13. Uchytíl P.: Použití anorganických a polymerních membrán pro pervaporaci. (Czech) Application of inorganic and polymeric membranes to pervaporation. *Chem. Listy* 94, 181-185 (2000).

Czech patents

14. Heyberger A., Tříška J., Bízek V.: Method and equipment for concentration of low-volatile substances. Czech. Pat. No. 286647 (2000).

Conferences

15. Hejtmánek V., Čapek P., Šolcová O., Uchytíl P.: Permeation of adsorbable gases in porous catalysts. 27th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 153, Tatranské Matliare, Slovakia, 22-26 May (2000).
16. Heyberger A., Volaufová E., Voborská J., Procházka J.: Extraction of tungsten with trialkylamine. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 180, Praha, 27-31 August (2000).
17. Hutton B., Heyberger A., Menu D., Godwin I., Myburg P.: Separation of phenolic derivatives by application of dissociation extraction. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. B7. 1, Praha, 27-31 August (2000).
18. Hutton B., Heyberger A., Myburgh P.: Dissociation extraction - theory and practical application. 9th International Meeting SAICHE 2000, Republic South Africa, 9-13 October (2000).
19. Jeřábek K., Hanková L., Prokop Z.: Morfologie zbotnalých hypersulfonovaných ionexových katalyzátorů. (Czech) Swollen-state morphology of hypersulfonated ion exchanger catalysts. 27th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 124, Tatranské Matliare, Slovakia, 22-26 May (2000).
20. Jeřábek K., Hanková L., Prokop Z.: Optimization of catalysts for bisphenol A synthesis. XXXIInd Symposium on Catalysis, p. Op7, Prague, 6-7 November (2000).
21. Jeřábek K., Hanková L., Prokop Z.: Hypersulfonated ion exchanger catalysts. 12th International Congress on Catalysis, Granada, Spain, 9-14 July (2000).
22. Jeřábek K., Hanková L., Prokop Z.: Hypersulfonated ion exchanger catalysts. 9th International Conference on Polymer Based Technology POC'2000, Tianjin, China, 21-26 May (2000).
23. Jeřábek K., Hanková L., Prokop Z.: Swollen-state morphology of hypersulfonated ion exchanger catalysts. Ion Exchange at the Millennium, ed. by Greig J. A., pp. 338-344 (Proceedings of IEX 2000), Churchill College, Cambridge, 16-21 July (2000).
24. Králík M., Zecca M., Biffis A., Jeřábek K., Corain B.: Generating palladium nanoclusters inside functional polymer networks: catalytic prospects. XXXIInd Symposium on Catalysis, p. Po11, Prague, 6-7 November (2000).
25. Ondráček J., Jiříčný V., Staněk V., Jakeš B.: RTD under counter-current gas-liquid flow in a column with packed and bubble bed in series. 4th International Scientific-Technical Conference Process Control 2000, Proceedings, p. 155, Kouty nad Desnou, Czech Republic, 11-14 June (2000).
26. Ondráček J., Jiříčný V., Staněk V., Svoboda P.: Hydrodynamics of packed bed and bubble bed columns in series. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 11, Praha, 27-31 August (2000).
27. Procházka J., Heyberger A., Volaufová E.: Extraction of dicarboxylic acids with tertiary amine in binary diluents. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 40, Praha, 27-31 August (2000).
28. Sovová H., Stateva R. P.: Effect of third component on the solubility of vegetable substances in supercritical CO₂. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 35, Praha, 27-31 August (2000).

29. Sovová H.: Solubility of natural products in SC CO₂ - data condensed with Adachi-Lu equation. 7th Meeting on Supercritical Fluids, Proceedings, p. 915, Antibes-Juan-les-Pins, France, 6-8 December (2000).
30. Svoboda P., Staněk V., Jiříčný V.: Transient states of the hydrodynamics of counter current flow in a packed bed near the flooding point. 4th International Scientific-Technical Conference Process Control 2000, Proceedings, p. 154, Kouty nad Desnou, Czech Republic, 11-14 June (2000).
31. Svoboda P., Ondráček J., Jiříčný V., Staněk V.: Experimental counter current packed bed column for complex measurement of hydrodynamics. 4th International Scientific-Technical Conference Process Control 2000, Proceedings, p. 156, Kouty nad Desnou, 11-14 June (2000).
32. Svoboda P., Staněk V., Jiříčný V., Ondráček J.: Transients of the hydrodynamics of packed bed gas-liquid column around the flooding point. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 10, Praha, 27-31 August (2000).
33. Uchytíl P., Thomas S., Seidel-Morgenstern A.: Flow direction dependence of vapor condensation in multilayer membranes. 6th International Conference on Inorganic Membranes, Book of Abstracts p. 129, Montpellier, France 26-30 June (2000).
34. Uchytíl P., Petříčkovič R.: Comparison of pervaporation of binary mixtures n-propanol-water and i-propanol-water through polyethylene membrane. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 101, Praha, 27-31 August (2000).
35. Veverka P., Jeřábek K.: Study of sorption properties of hypercrosslinked polymer sorbents. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 269, Praha, 27-31 August (2000).
36. Volaufová E., Heyberger A., Procházka J.: Extraction of succinic acid. 27th International Conference of Slovak Society of Chemical Engineering, Tatranské Matliare, Slovak Republic, 22-26 May (2000).
37. Vychodilová H., Staněk V., Jiříčný V.: Absorption of poorly soluble gases in co-current packed bed column by transient technique. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 2, p. 13, Praha, 27-31 August (2000).

E. Hála Laboratory of Thermodynamics

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

Fields of research

- Determination of fluid phase equilibrium data at low, normal, and high pressures
- Experimental determination and molecular modelling of phase equilibria in systems with chemical reaction
- Determination of pressure–volume–temperature behaviour of liquids
- Thermodynamic modelling and processing of thermodynamic data
- Development of equations of state based on molecular theory
- Molecular simulations on model fluids and fluid mixtures
- Application of statistical–mechanical models to real fluids
- Molecular modelling of solubility of liquids
- Theory of polar compounds
- Study of hydrophobic interactions
- General phase behaviour of binary mixtures – global phase diagrams
- Compilation of bibliographic information on vapour–liquid equilibrium data

Applied research

- Computerized bibliography of vapour–liquid equilibrium data

Research projects

Equations of state for real non-simple fluids and their mixtures, based on molecular theory

(K. Aim, supported by GA ASCR, grant No. A4072712)

Study on homo- and hetero-nuclear square-well diatomic fluids by Monte Carlo simulations and integral equation theory has been completed. Further investigations conducted were aimed at (i) improving the performance of an equation of state based on the two-centre Lennard–Jones dipolar model fluid, (ii) developing and testing equations of state (based on primitive model of association) for real systems containing associating fluids, and

(iii) applications of the RGEMC method to calculating phase equilibrium in binary systems representing different types of interactions. [Refs. 1, 3, 4, 15, 16, 17, 23, 34]

Phase and state behaviour of fluid systems

(K. Aim, joint project with ICT; supported by GA CR, grant No. 104/99/0136)

Experimental studies on relevant pure-compound vapour pressures (by high precision comparative ebulliometry) and on vapour–liquid equilibria (by dynamic still) have continued for a series of binary and ternary systems of the type ether + alkanol + hydrocarbon. New equilibrium cell for static measurements has been constructed. Applicability of gnostic theory to critical evaluation of high-pressure vapour-liquid equilibrium data has been examined. Supplement to the vapour–liquid equilibrium data bibliography has been completed. [Refs. 8, 10, 11, 12, 22, 25, 35, 38, 40]

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

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

The recently assembled apparatus for the measurement of densities of liquid mixtures in the range from normal to high pressures has been used to determine excess volume data at normal pressure from 298 to 328 K for binary systems of the type heptane plus linear 1-chlorohydrocarbon (C₄ to C₆) and to re-measure the densities of n-heptane + 1-chloropentane mixtures at temperatures up to 330 K and pressures up to 400 bar. The perturbation theory for fluids constituted of anisotropic molecules has been examined by using the newly available excess property data for systems of the alkane + (chloro-)alkane type. [Refs. 14, 19, 30, 32]

From simple models toward molecular theory of associated liquids. Theory and application

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

Very extensive computer simulations have been carried out to examine in detail the effect of the range of intermolecular interactions on the orientation arrangement both in water and other associating fluids and polar fluids. [Refs. 2, 6, 7, 18, 20, 29]

Behaviour of liquids at very high pressures: Theory and applications

(I. Nezbeda, joint project with ICT, supported by GA CR, grant No. 203/99/0134)

Accuracy of a suitably chosen reference system was tested along with a new equation of state for a binary mixture of additive hard spheres with the focus on demixing conditions. General rules leading to a new family of molecular-based equations of state have been formulated and individual steps tested. [Refs. 2, 5, 9, 13, 16, 17, 27, 33, 34]

Molecular thermodynamics of polar and associating fluid mixtures

(Co-researchers: J. Fischer (Institute of Environmental and Energy Engineering, University of Agricultural Sciences, Vienna) and I. Nezbeda; supported by AKTION – The Czech-Austrian co-operation program 1999-2001)

Investigations continued to pursue two paths. (1) Study of systems of dipolar two-center Lennard–Jones fluids. A project to obtain new and more accurate computer simulation data has been launched. (2) Steps leading ultimately to a new equation of state for the class of associating fluids have further been examined. An equation of state for water has been formulated and its accuracy and applicability is being tested. [Refs. 3, 39]

Phase equilibria in systems with chemical reaction

(I. Wichterle, supported by GA CR, grant No. 203/98/1446)

Vapour–liquid equilibria were studied in systems where chemical reaction takes place. Another esterification reaction namely acetic acid + ethyl alcohol \rightleftharpoons ethyl acetate + water was measured at isothermal conditions. A good prediction of both the chemical and phase equilibria was achieved with use of data for binary subsystems while parameters for reacting systems (alcohol + acid, water + ester) were adjusted from quaternary data. A newly proposed simulation method (Reaction Ensemble Monte Carlo) has also been used for evaluation of thermodynamic properties of plasma systems (helium, argon, air). [Refs. 4, 5, 15, 21, 24, 26, 31, 32, 36, 37, 41]

International co-operations

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

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

Sonderforschungsbereich, University of Leipzig, Leipzig, Germany: Fluid in confined geometry

Novo Nordisk, Denmark: Study of proteins by the essential dynamics method

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

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

Northwestern University, Evanston IL, USA: Polarizable models of salt melts

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

Visits abroad

M. Lísal: University of Guelph, Guelph, Canada (3 months)

M. Lísal: North Carolina State University, Raleigh NC, USA (4 months)

I. Nezbeda: University of Tennessee, Knoxville TN, USA (4 months)

M. Předota: University of Tennessee, Knoxville TN, USA (12 months)

Visitors

J. P. O'Connell, University of Virginia, Charlottesville VA, USA

J. Fischer, University of Agricultural Sciences, Vienna, Austria

E. B. Smith, University of Melbourne, Australia

W. R. Smith, University of Guelph, Guelph, Canada

H. L. Vörtler, University of Leipzig, Leipzig, FRG

U. Weingerl, University of Agricultural Sciences, Vienna, Austria

Teaching

- J. Kolafa and I. Nezbeda: CU, course: "Introduction to computer simulations in many particle systems"
- I. Nezbeda: Purkyně University, courses: "Analytical mechanics", "Introduction to computer simulations", "Mathematics for physicists", "Thermodynamics and statistical physics"
- I. Nezbeda, K. Aim: ICTP, postgraduate course "Applied statistical thermodynamics of fluid systems"

Publications

Papers

1. Jirásek V., Labík S., Malíjevský A., Lísal M.: An integral equation and Monte Carlo study of homo-and hetero-nuclear square-well diatomic fluids. *Mol. Phys.* 98, 2033-2044 (2000).
2. Kolafa J., Nezbeda I.: Effect of short and long range forces on the structure of water. II. Orientational ordering and the dielectric constant. *Mol. Phys.* 98, 1505-1520 (2000).
3. Lísal M., Aim K., Fischer J.: Vapour-liquid equilibria of dipolar two-centre Lennard-Jones fluids from a physically based equation of state and computer simulations. *Mol. Sim.* 23, 363-388 (2000).
4. Lísal M., Smith W. R., Nezbeda I.: Molecular simulation of multicomponent reaction and phase equilibria in MTBE ternary system. *AIChE J.* 46(4), 866-875 (2000).
5. Lísal M., Smith W. R., Nezbeda I.: Computer simulation of the thermodynamic properties of high-temperature chemically-reacting plasmas. *J. Chem. Phys.* 113(12), 4885-4895 (2000).
6. Nezbeda I.: Solubility of apolar fluids in water: a simple molecular model and theory. *Fluid Phase Equilib.* 170, 13-22 (2000).
7. Nezbeda I.: On the role of short-and long-range forces in aqueous systems. *J. Mol. Liq.* 85, 249-255 (2000).
8. Roháč V., Čenský M., Zala D., Růžička V., Růžička K., Sporka K., Aim K.: Vapor pressure and liquid heat capacity of perhydroacenaphthylene and perhydrophenanthrene. *J. Chem. Eng. Data* 45(6), 1205-1210 (2000).
9. Strnad M., Nezbeda I.: Parallelized sampling of the Gibbs ensemble. *Mol. Phys.* 98(22), 1887-1984 (2000).
10. Teodorescu M., Wagner Z., Wichterle I.: Application of the predictive UNIFAC model to the pentan-3-one/chloroalkane and 5-chloro-2-pentanone/hydrocarbon binary systems. *Chem. Eng. Technol.* 23(4), 367-370 (2000).
11. Teodorescu M., Wichterle I.: Evaluation of the carbonyl/chlorine interaction parameters in pentan-3-one-chloroalkane mixtures using the DISQUAC group contribution model. *Collect. Czech. Chem. Commun.* 65(10), 1559-1572 (2000).
12. Bernatová S., Wichterle I.: Isothermal vapour-liquid equilibria in the ternary system tert-butyl methyl ether + tert-butanol + 2,2,4-trimethylpentane and the three binary subsystems. *Fluid Phase Equilib.* (in press).
13. Kettler M., Strnad M., Nezbeda I., Vörtler H. L.: Coexistence properties of higher n-alkanes modeled as Kihara fluids: Gibbs ensemble simulation. *Fluid Phase Equilib.* (in press).
14. Kovács É., Linek J.: Excess molar volumes of (alkane+1-chloroalkane) at T = 298.15 K. *J. Chem. Thermodyn.* (in press).

15. Lísal M., Smith W. R., Nezbeda I.: Accurate vapor-liquid equilibrium calculations for complex systems using the Reaction Gibbs Ensemble Monte Carlo simulation method. *Fluid Phase Equil.* (in press).
16. Nezbeda I.: On molecular-based equations of state. Rigor versus speculations. *Fluid Phase Equil.* (in press).
17. Nezbeda I.: On dispersion forces correction terms in perturbed equations of state. *Fluid Phase Equil.* (in press).
18. Nezbeda I., Lísal M.: Effect of short-and long-range forces on the thermodynamic properties of water. A simple short-range reference system. *Mol. Phys.* (in press).
19. Pavlíček J., Boublík T., Aim K.: Fluids of the Kihara molecules II. Binary mixtures of n-alkanes. *J. Phys. Chem.* (in press).
20. Slovák J., Tanaka H., Koga K., Zeng X. C.: Computer simulation of water-ice transition in hydrophobic nanopores. *Physica A* (in press).
21. Teodorescu M., Aim K., Wichterle I.: Isothermal vapor-liquid equilibrium in the quaternary water + isopropanol + acetic acid + isopropyl acetate system with chemical reaction. *J. Chem. Eng. Data* (in press).

Monographs

22. Wichterle I., Linek J., Wagner Z., Kehiaian H. V.: Vapor-liquid equilibrium in mixtures and solutions. *Bibliographic Database EVLM'2000. Integrated Electronic Chemical Databases*, 285 pp. + CD-ROM, ELDATA, Paris (2000).

Conferences

23. Aim K., Lísal M., Smith W. R.: Molecular simulation of vapour-liquid equilibria in some binary systems with specific interactions. 18th European Seminar on Applied Thermodynamics ESAT 2000, Conference Book, p. 172, Kutná Hora, Czech Republic, 8-11 June (2000).
24. Aim K., Teodorescu M., Wichterle I.: Vapour-liquid equilibrium in a quaternary system with esterification reaction: measurement and data correlation. 18th European Seminar on Applied Thermodynamics ESAT 2000, Conference Book, p. 49, Kutná Hora, Czech Republic, 8-11 June (2000).
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Department of Catalysis and Reaction Engineering

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

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

Applied research

- Catalytic combustion of volatile organic compounds

Research projects

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

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

The standard textural analysis methods (the nitrogen physisorption, mercury porosimetry, helium pycnometry, and liquid-expulsion permoporometry) and non-standard transport measurement methods (multicomponent counter-current isobaric diffusion, gas permeation under non-steady state conditions) are applied for complex analysis of pore structure of a broad set of industrial porous solids (monodisperse pore-size distributions, bi- and polydisperse pore-size distributions, with micropores, mesopores and macropores, etc.). The correlation of data obtained from all methods allow a novel approach in determination and prediction of transport parameters characterizing processes taking place in porous solids (porous heterogeneous catalysts, membranes, adsorbents, zeolites etc.). [Refs. 4, 15, 25, 36, 51, 52, 54]

Graham cell for multicomponent gas diffusion in porous solids

(P. Schneider, supported by GA ASCR, grant No. 4072804)

A version of the Wicke-Kallenbach diffusion cell that utilizes the validity of Graham law to simplify the cell construction and operation is studied and developed. A numerical algorithm is set up for evaluation of parameters of the Mean Transport-Pore Model; these parameters are material constants of the porous solids, i.e., are independent of the measurement conditions and kind of diffusion gases. To increase the confidence of model parameters obtained from diffusion measurements, we have enlarged the volume of experimental information by performing counter-current diffusion measurements with multicomponent gas mixtures. [Refs. 26, 37, 53]

Strengthening of national capabilities in assessment of the NPP civil structures for regular purposes

(O. Šolcová, co-operation with the Faculty of Civil Engineering of the Czech Technical University in Prague, supported by International Atomic Energy Agency Vienna, Austria, grant No. CZR9011-04447J)

A set of criteria on the durability of concrete containment structures for nuclear safety assessment purposes is defined. The concrete samples of Temelin (Czech Rep.) and Penly (France) are used for physical testing the persistence of the concrete structures from the both localities. Texture properties of concretes are determined by mercury porosimetry and physisorption of inert gases.

Heterogeneous catalysts and catalysts precursors of monolayer type: new type of synthesis by "slurry impregnation method"

(M. Zdražil, supported by GA ASCR, grant No. A4072802)

The new "slurry impregnation" method was applied for preparation of supported MoO₃ catalysts. The catalysts were tested in hydrodesulfurization of model compounds and were compared with industrial MoO₃/Al₂O₃ catalysts. High activity MoO₃/MgO catalysts were prepared by the reaction of high surface area MgO with the slurry of (NH₄)₆Mo₇O₂₄ or MoO₃ in methanol or ethanol [Refs. 5, 17, 30, 41, 42]. In that case, the "slurry impregnation" in non-aqueous environment overcomes the chemical and textural instability of high surface area MgO in conventional aqueous impregnation. Active carbon supported MoO₃ catalysts were prepared by adsorption of MoO₃ from the slurry MoO₃/water. Very high loadings of about 30% were achieved and calcination was not needed [Refs. 16, 39, 40]. The results achieved by the "slurry impregnation" in the group up to now were summarised and discussed [Ref. 28].

Iridium promoted molybdenum sulphide hydrodenitrogenation catalysts

(Z. Vít)

The Mo/Al₂O₃ catalyst was modified by iridium and tested in hydrodenitrogenation (HDN) of pyridine and hydrodesulfurization (HDS) of thiophene. Iridium had positive effect on both HDN and HDS. A synergetic effect between Mo and Ir was observed in HDN (three times) at about 0.3-0.5 wt. % Ir. Results of H₂ adsorption on the reduced catalysts and TPR of sulfided catalysts confirmed an interaction between Ir and Mo, resulting in higher reducibility and activity of modified catalysts. The results of H₂ adsorption and TEM suggest that dispersion of the promoter is more important than its amount [Refs. 3, 27]. Relation between reducibilities of oxidic precursors and sulfide catalysts are discussed [Ref. 55].

Catalytic combustion of volatile organic compounds

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

Catalytic combustion of model organic compounds (toluene, ethanol) was studied with respect to the catalyst composition and the way of its preparation. In preparation of Pt

catalysts, effect of microemulsion composition and Pt concentration on catalytic activity in VOC combustion was examined. Supported salts of phosphomolybdic acids and calcined hydrotalcite-like compounds containing various combinations of transition metal oxides were prepared and characterized from the point of view of their physical chemical properties and catalytic activity in combustion of VOC. [Refs. 10, 19, 23, 35, 48, 49]

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

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

Zirconium containing mesoporous silicas were prepared and used as new supports of HDS catalysts. Nickel introduced as a counter-cation of HPMo in NiMo/HMS catalyst stabilized the Keggin structure of HPMo. Zirconium in the support favours lacunar anion formation as a result of interaction between molybdenum compound and support in NiMo/Zr-HMS catalysts. Nickel also makes molybdenum reduction of NiMo/Zr-HMS easier. Catalytic activities in hydrodesulphurization (HDS) of thiophene of the molybdenum containing catalysts prepared with the hexagonal mesoporous silicas were higher than the activity of the catalyst prepared with amorphous silica. Nickel introduced as counter-cation of Keggin structure of heteropoly anion enhanced and stabilized the HDS activity. [Refs. 18, 24, 43, 44, 50]

Role of electron pairing in chemical bonds

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

The project deals with the application and exploitation of pair density as a new means of analysis of the role of electron pairing in chemical bonds. The main goal of the project is to extend the previous author's studies applied so far to ground states of closed-shell molecules to other systems like open-shell molecules, radicals, biradicals, molecules in excited states, metallic clusters, etc. In addition to this, the attention is also devoted to further methodological development of the alternative methods of analysis of pair density and/or related quantities. Especially promising seem to be, in this respect, the so-called Fermi-holes and their analysis as a new source of structural information is also be systematically pursued. [Refs. 1, 2, 6, 8, 9, 13, 14, 20, 21, 22, 31, 32, 33]

Design of theoretical QSAR models based on quantum similarity data

(R. Ponec, supported by grant Ministry of Education, D0.20)

The project deals with the application of similarity measures and indices, derived from quantum chemically generated density matrices, as new universal molecular descriptors for the design of theoretical QSAR models in rational drug design. This project is solved in close collaboration with the Institute of Computational Chemistry of the University of Girona which has a long term expertise in the design of quantum similarity data and the results of the collaboration in the year 2000 are summarized in the studies. [Refs. 7, 11, 12, 44]

International co-operations

Analysis of the pair density matrix: University of Liverpool, Liverpool, UK; University of Hannover, Hannover, Germany; University of Buenos Aires, Buenos Aires, Argentina; Institute of Computation Chemistry, University of Girona, Spain; University of Pais Vasco, Bilbao, Spain

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

Effect of acidity of a support on VOC oxidation over supported metal catalysts. ICE-HT/FORTH, Patras, Greece

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

Visits abroad

R. Ponec: University of Girona, Spain (3 months)

Visitors

V. Vishwanathan, Indian Institute of Chemical Technology, Hyderabad, India (1 month)

Teaching

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

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

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

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

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17. Klicpera T., Zdražil M.: High surface area MoO₃/MgO: Preparation by reaction of MoO₃ and MgO in methanol or ethanol slurry and activity in hydrodesulphurization of benzothiophene. *Appl. Catal., A* (in press).
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Department of Multiphase Reactors

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

Fields of research

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

Research projects

Hydrodynamic instabilities in bubble column reactors

(M. Růžička, supported by GA CR, grant No. 104/98/1435)

Studies of transition between homogeneous and heterogeneous flow regimes in bubble columns. The identification of hydrodynamic mechanisms causing the instability of the homogeneous bubbling regime, investigation of the character of this instability. [Refs. 4, 5, 10, 11, 18, 26-29]

Increasing the transport coefficients of convective processes by means of jet flow modulation

(V. Sobolík, joint project with CTU, Faculty of Mechanical Engineering, Prague; supported by GA CR, grant No. 101/99/0060)

Convective heat and mass transfer between the fluid jet and the wall placed opposite the impinging jet have been investigated experimentally with the aim to achieve the increase in the value of transfer coefficient by means of applying a periodic modulation of the flow from the nozzle of supply.

Electrochemical sensors for flow measurements

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

Electrochemical technique for the near-wall flow diagnostics has been improved (sensors manufacturing, development of the control electronics, dynamic response of the sensors). The directionally sensitive segment probes have been applied to study different flow situations (near-wall turbulence, backward-facing step flow, Taylor-Couette flow, impinging fluid jet). [Refs. 6, 13]

The evolution of surface waves in film flow down an oscillating inclined plane

(J. Tihon, supported by GA ASCR, grant No. A4072914)

The stability of the Newtonian film flowing down an oscillating wall has been studied with the aim to predict the effect of parallel wall oscillations on the flow character in the liquid film. The linear stability analysis has provided the criterion for wave inception and the estimation of wave growth rates for different oscillation regimes (film flow stabilization or destabilization). The following experiments (film thickness and wall shear stress measurements) will cover a wide range of the operation parameters: flow rate, inclination angle, liquid properties, and parameters of oscillations. [Refs. 30-32]

Evaluation of a new energy-saving mixing impeller for the process industries

(M. Fialová, joint project with UMIST Manchester, UK, Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria, Aristotle University Thessaloniki, Greece and Performance Fluid Dynamics Ltd, Dublin, Ireland; supported by the Commission of the European Communities under INCO-COPERNICUS contract No. IC15-CT98-0502.)

An extensive programme of visualisation experiments has been accomplished, aimed at determining gas-flow patterns in bubble columns at different modes of primary gas distribution. Resulting video-images were used for the verification of the cellular automata model proposed previously for modelling of gas-liquid flow in bubble column reactors and for the two-loop circulation model employed as a starting assumption in derivation of the network-of-zones model for bubble column reactors. The network-of-zones model was applied for the prediction of gas hold-up in bubble column reactors and for interpretation of the results of plant trials performed in an industrial bubble column fermentor. An experimental study of bubble coalescence in aqueous media has been carried out in a coalescence cell with the purpose of further examining the contradictory effects of viscosity and surface activity on bubble coalescence. [Refs. 1, 2, 7, 14, 20-23, 33, 37, 38]

Modelling and design of multiphase bubble-bed reactors for advanced food-industry technologies

(M. Růžička, joint project with Aston University, Birmingham, UK, University of Minho, Braga, Portugal, Slovak Technical University, Bratislava; supported by the Commission of the European Communities under COPERNICUS contract No. IC15-CT98-0904).

Studies on (i) basic experimental and theoretical hydrodynamics of two-phase bubble beds including effects of viscosity, surface tension, and presence of third phase, (ii) oxygen transfer in bubble-beds, (iii) hydrodynamics of real fermentors as used in food-industry, (iv) CFD simulation of model and real multiphase flows, (v) modelling and improving real reacting systems. [Refs. 4, 5, 10, 11, 18, 26-29]

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

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

The project gives young researchers pursuing doctoral studies the opportunity to receive training within diagnostics of multiphase flows. Four specialized vacancies are suggested for the current academic year.

Rheometric and electrodiffusion study of the apparent slip in lyophilic dispersions

(O. Wein, internal project of ICPF, 2000)

Apparent wall slip in several water-soluble polysaccharides was studied experimentally, using rotational viscometry. An extensive collection of the related material functions has been obtained. Viscometric theory was developed for a novel rotational viscometer with coaxial Morse cones. [Refs. 34-36]

International co-operations

University of Tokyo, Tokyo, Japan: Chaotic hydrodynamics of bubble columns
Aston University, Birmingham, UK: Multiphase chemical reactors and bioreactors
UMIST, Manchester, UK: Gas-liquid reactors for complex rheology fluids
University of Minho, Braga, Portugal: Multiphase bubble bed reactors
CNRS UPR 15, Paris, France: Electrodiffusion diagnostics of flow
CRTT, Saint Nazaire, France: Backward-facing step flows
LEMTA, INPL, Vandoeuvre les Nancy, France: Ekman vortices
LEGI / IMG, Grenoble, France: Impinging jets
University of Poitiers, France: Electrochemical sensors for flow measurements
Institute of Chemical Engineering, BAS, Sofia, Bulgaria: Gas-liquid reactors for complex rheology fluids
University of Sao Paulo, Sao Paulo, Brazil: Application of neural network in two-phase flow
Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow
University of Thessaly, Volos, Greece: Liquid film flows

Visits abroad

M. Růžička: DAMTP, University of Cambridge, UK (2 months)
V. Sobolík: University of La Rochelle, France (12 months)
J. Vejražka: LEGI / IMG, Grenoble, France (6 months)

Visitors

V. Bontozoglou, University of Thessaly, Volos, Greece
W. Bujalski, University of Birmingham, UK
C. Deslouis, CNRS, UPR 15, Paris, France
H. Iwata, NIRE, Tsukuba, Japan
H. M. Nagib, Illinois Institute of Technology, Chicago, USA
A. W. Nienow, University of Birmingham, UK
J. A. Teixeira, University of Minho, Braga, Portugal
N. H. Thomas, Aston University, Birmingham, UK
S. D. Vlaev, Institute of Chemical Engineering, BAS, Sofia, Bulgaria

Teaching

J. Drahoš: ICT, course "Fluid Mechanics" and postgraduate course "Multiphase reactors"

J. Tihon: ICT, postgraduate course "Drops, bubbles and particles"
O. Wein: TU Brno, course "Principles of Rheology"

Publications

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2. Havelka P., Linek V., Sinkule J., Zahradník J., Fialová M.: Hydrodynamic and mass transfer characteristics of ejector loop reactors. *Chem. Eng. Sci.* 55(3), 535-549 (2000).
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4. Růžička M.: On bubbles rising in line. *Int. J. Multiphase Flow* 26, 1141-1181 (2000).
5. Růžička M., Drahoš J., Zahradník J., Thomas N. H.: Structure of gas pressure signal at two-orifice bubbling from a common plenum. *Chem. Eng. Sci.* 55(2), 421-429 (2000).
6. Sobolík V., Izrar B., Lusseyran F., Skali S.: Interaction between the Ekman layer and the Couette-Taylor instability. *Int. J. Heat Mass Transfer* 43(24), 4381-4393 (2000).
7. Vlaev D., Mann R., Lossev V., Vlaev S. D., Zahradník J., Seichter P.: Macro-mixing and *Streptomyces fradiae* modelling oxygen and nutrient segregation in an industrial bioreactor. *Trans IChemE* 78, Part A, 354-362 (2000).
8. Vrba J., Punčochář M., Drahoš J.: Fuzzy decomposition applied on logistic equation. *SAMS* 38, 65-80 (2000).
9. Vrba J.: Standardized procedures in fuzzy modelling and simulation of complex recycle processes. *SAMS* 37, 359-379 (2000).
10. Růžička M., Zahradník J., Drahoš J., Thomas N. H.: Homogeneous-heterogeneous regime transition in bubble columns. *Chem. Eng. Sci.* (in press).
11. Růžička M., Thomas N. H., Zahradník J., Drahoš J.: Convective instability of a uniform horizontal bubbly layer confined by vertical walls. *Int. J. Multiphase Flow* (in press).
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14. Zahradník J., Mann R., Fialová M., Vlaev D., Vlaev S. D., Lossev V., Seichter P.: A networks-of-zones analysis of mixing and mass transfer in three industrial bioreactors. *Chem. Eng. Sci.* (in press).

Czech patents

15. Hájek M., Drahoš J.: Způsob a zařízení k tepelnému zpracování přírodních materiálů, zvláště vulkanického původu. (Czech) Method and apparatus for heat treatment of glass materials and natural materials specifically of volcanic origin. *Czech. Pat. PV 2000-1935* (in press).

International patents

16. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and apparatus for heat treatment of glass materials and natural materials specifically of volcanic origin. PCTI/CZ00/00042/ (in press).

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18. Drahoš J., Růžička M.: From a bubble to bubble columns. 2nd Japanese-European Two-Phase Flow Group Meeting, Abstracts, p. J-1, Tsukuba, Japan, 25-29 September (2000).
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21. Fialová M., Zahradník J., Vlaev D. S., Mann R., Seichter P.: Application of the network-of-zones model for calculation of local hydrodynamic parameters of a bubble column fermentor. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 1, p. 167, Praha, 27-31 August (2000).
22. Freitas C., Fialová M., Zahradník J., Teixeira J. A.: Comparative evaluation of the hydrodynamics of an external - and an internal - loop airlift reactor for three-phase systems. 27th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 53, Tatranské Matliare, Slovakia, 22-26 May (2000).
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25. Jochová M., Horáček J., Punčochář M., Drahoš J.: Recovery of heavy metals from waste water. International Workshop on Effective Utilization of Waste for Minimum Emission and its Safety, Proceedings, pp. 87-93, Kraków, Poland, 7-9 March (2000).
26. Nascimento C. A. O., Drahoš J., Guardani R., Růžička M., Lubbert A.: Use of neural network for identification of bubbling mode from a submerged orifice. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 3, p. 131, Praha, 27-31 August (2000).
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- International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 107, Tatranské Matliare, Slovakia, 22-26 May (2000).
29. Růžička M., Zahradník J., Drahoš J., Fialová M., Thomas N. H.: Effect of bubble column size on homogeneous regime stability. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 3, p. 125, Praha, 27-31 August (2000).
 30. Thin J., Tovčigrečko V. V.: Nová modelová elastická kapalina připravená na bázi vodorozpustných polymerů. A new model-elastic liquid based on water-soluble polymers. 27th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 119, Tatranské Matliare, Slovakia, 22-26 May (2000).
 31. Thin J., Pěnkavová V., Sobolík V., Wein O.: Surface waves artificially forced on flowing liquid films. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 3, p. 139, Praha, 27-31 August (2000).
 32. Thin J., Wein O.: Wave instabilities in non-Newtonian liquid films. XIIIth International Congress on Rheology, Proceedings, p. 3-216-3-218, Cambridge, UK, 20-25 August (2000).
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 34. Večeř M., Tovčigrečko V. V., Wein O.: Viskometria potravinářských kvapalín pri zdánlivom skluzе. The viscometry of food fluids under apparent wall slip. 27th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 126, Tatranské Matliare, Slovakia, 22-26 May (2000).
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Department of Biotechnology and Environmental Processes

Head: J. Čermák
Deputy: M. Hájek
Research staff: T. Brányik, V. Církva, M. Czakoová, V. Gruber, J. Hájek, J. Hetflejš,
J. Houferák, F. Kaštánek, D. Klier, G. Kuncová, Y. Maléterová,
H. T. T. Nguyen, J. Szilva, S. Šabata, J. Včelák
Part time: L. Fiala, O. Podrazký, H. Sándorová
Technical staff: K. Auerová, J. Brustman, Z. Soukup, J. Storch, J. Tschackert
PhD students: J. Kurfürstová, M. Prajzlerová, L. Šťastná

Fields of research

- Aerobic bioreactor with immobilized cells - design and scale-up
- Bioremediation of organic pollutants in soil and sewage
- Immobilization of biocatalysts, development of new agents for their chemical bonding to inorganic supports
- Optical fibre sensors for chemical reactors, monitoring of water and soil pollution
- Detoxification of noxious halogen-containing substances by chemical and biochemical dehalogenation
- Microwave-induced catalytic reactions
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphasic media
- Chemical modification of telechelic polybutadienes and synthesis of triblock siloxane-butadiene copolymers

Applied research

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

Research projects

Revaluation of dangerous waste on the basis of ferric oxides with portion of heavy metals (furnace steel dusts) as a new additive to building materials

(F. Kaštánek, project supported by GA CR, grant No.104/99/0440)

The project objective is to clarify and theoretically justify the positive impact of addition of ferric oxide particles of average size under 1 μm on the properties of materials on the basis of cement (increase of liquidity of cement mixtures, increase of strength and water resistance

of mortars and concretes, and increase of their corrosion resistance to chemical and physical effects of environment). The project deals also with very topical practical problems of disposal of waste by the most convenient way (both ecologically and economically) of using waste as a basic component of building materials with improved and health not affecting properties. Current state of knowledge gained in our project could be summarised as follows: if cement is replaced by furnace steel dust (up to approx. 15 %w/w) a considerable increase of the strength of products – mortars and/or concretes and higher frost resistance in comparison with concretes without these additives occur. The important finding of our research is also the fact that hazardous waste can be immobilised in this way in the form harmless to human health, which meets legal hygiene norms valid in the Czech Republic. [Ref. 20]

Biodegradation of phenols in water and water sediments

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

The efficiency of biodegradation of phenols adsorbed on real contaminated sediments depends on the size of sediments particles, physico-chemical characteristics of individual types of sediments and bioavailability of organic phase to microorganisms. Knowledge of basic decisive mechanisms of biodegradation at real natural condition is essential not only from the viewpoint of bringing new scientific understanding, but also regarding the selection and design of the bioreactor configuration. The aim of project is to elucidate the pathways of biodegradation of individual selected strain of microorganisms and to propose realistic bioreactor configuration for effective biodegradation of naturally contaminated sediments and underground waters.

Novel techniques for implementation of immobilized biocatalysts in industrial processes

(G. Kuncová, supported by INCO-COPERNICUS project Erbic15CT98, and Ministry of Education of the Czech Republic)

The main objective of this project, which started in October 1998, is to facilitate the implementation of new materials and techniques into industrial biocatalytic processes. The project is a concerted action involving multidisciplinary, trans-national teams, to integrate the expertise on immobilized biocatalysts. [Refs. 40, 42, 44]

Bioencapsulation innovation and technologies

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

The Action aims to foster co-operation in Europe, in part through yearly meetings and scientific contribution to international conferences, in research and development of bioencapsulation technologies, in order to: (a) increase the awareness of possibilities offered by the new materials in the biocatalyst encapsulation, (b) identify new processes allowing use of these materials under mild and biocompatible conditions, (c) collaborate to develop and test the encapsulation processes on large scale, (d) characterise and optimise the microcapsule materials and the related processes to suit the requirements of specific applications in biotechnology, agriculture and nutrition, (e) evaluate the different applications of biocapsules in terms of economy, (f) identify industrial partners and involve them in Action.

In ICPF the research is focused on encapsulation by sol-gel technique and development of optical monitoring of immobilized living cells. A comparative study of phenol degrading cells immobilized by sol-gel method into silica gel and that cells immobilized by different technique, e.g. adsorption on ceramic surface or entrapment in polyurethane foam was finished. The method of estimation of cell viability using fluorescent spectrophotometer with optical fibres was developed and compared with viability measurement by fluorescent microscopy. [Refs. 1, 2, 11, 12, 21]

Microwave activation of heterogeneous catalytic reactions

(M. Hájek)

Research has been focused on microwave activation of heterogeneous catalytic reactions in liquid phase. It was found on model reaction of transformation of t-butylphenols that microwaves have a strong effect on reaction rate and selectivity. The results were explained on the basis of microwave-controlled transition state reactivity and microwave directed transition state selectivity. [Refs. 8, 16, 32, 36-39, 43]

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. [24, 26-29, 34, 35-39]

Liquid polybutadienes, their chemical modifications, block copolymers and organized structures

(J. Hetflejš, joint project with Institute of Macromolecular Chemistry ASCR, supported by GA ASCR, grant No. 4072902)

Chemical modifications of liquid polybutadienes are investigated using reactions leading to the introduction of reactive groups (e.g. alkoxy-silyl, hydroxy, isocyanato) via 1,2-additions to side polymer chains with the purpose of preparing novel materials for chemical specialties research. Also studied are several synthetic routes to triblockpoly(dimethylsiloxane)-butadiene copolymers to afford models for studies of mesoscopic structures.

Transition metal complexes with cyclopentadienyl ligands for catalysis in fluoruous biphasic systems

(J. Čermák, joint project with ICT, supported by GA CR, grant No. 203/99/0135)

Partition coefficients of novel perfluoroalkyl-substituted tetramethylcyclopentadienes (Cp^fH) together with their rhodium(III) and rhodium(I) complexes of the types $[\text{Cp}^f\text{RhCl}_2]_2$ and $[\text{Cp}^f\text{RhL}_2]$ were measured. X-ray structure of the Rh(III) chloro complex $[\text{Cp}^f\text{RhCl}_2]_2$ ($\text{Cp}^f = \text{C}_5\text{Me}_4\text{C}_6\text{F}_{13}$) was determined as the first known of its kind. Synthesis of cyclopentadienes substituted with one or two polyfluoroalkyl chains, $\text{C}_5\text{H}_{6-n}(\text{CH}_2\text{CH}_2\text{R}^f)_n$ and $(\text{Me}_3\text{Si})_{3-n}\text{C}_5\text{H}_3(\text{SiMe}_2\text{CH}_2\text{CH}_2\text{R}^f)_n$ ($n = 1, 2$), was accomplished. These compounds represent "second generation" of ligand precursors for catalysis by transition metal complexes in fluoruous biphasic media. [Ref. 30]

International co-operations

Université de Paris-Sud, Paris, France: Microwave activation of solvent-free reactions

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

Institute National Polytechnique de Lorraine Ecole National Supérieure d'Agronomie et des Industries Alimentaires (ENSAIA), Nancy, France: Alginate beads coated with silica layer

Visits abroad

V. Církva: University of Madison, Madison, USA (5 months)

J. Hetflejš: University of Arizona, Tucson; Stanford University, Stanford; Lawrence Livermore National Laboratory, Livermore, USA (3 weeks)

Visitors

F. Almeida, Instituto Superior Técnico, Lisbon, Portugal (5 weeks)

Teaching

F. Kaštánek: TU Brno and ICT: course "Bioengineering"

Publications

Papers

1. Brányik T., Kuncová G.: Changes in phenol oxidation rate of a mixed microbial culture caused by sol-gel immobilization. *Biotechnol. Lett.* 22(7), 555-560 (2000).
2. Brányik T., Kuncová G., Páca J.: The use of silica gel prepared by sol-gel method and polyurethane foam as microbial carriers in continuous degradation of phenol. *Appl. Microbiol. Biotechnol.* 54(2), 168-172 (2000).
3. Carvalho M. F. N. N., Duarte M. T., Galvao A. M., Pombeiro A. J. L., Čermák Jan, Šabata S., Vojtíšek P., Podlaha J.: Activation of a coordinated alkyne by electron transfer. Crystal structures of $[\text{Pd}\{\text{PPh}_2\text{CH}-\text{C}(\text{But})\text{NN}=\text{C}(\text{But})\text{CH}_2\text{PPh}_2\}\{\text{C}(\text{CO}_2\text{Me})=\text{CH}(\text{CO}_2\text{Me})\}]$ and $[\text{Pd}\{(Z,Z)\text{PPh}_2\text{CH}_2\text{C}(\text{But})=\text{NN}=\text{C}(\text{But})\text{CH}_2\text{PPh}_2\}\{\text{C}(\text{CO}_2\text{Me})=\text{C}(\text{CO}_2\text{Me})\}]$. *J. Organometal. Chem.* 598, 318-328 (2000).
4. Církva V., Gaboyard M., Paleta O.: Fluorinated epoxides. 5. Highly selective synthesis of diepoxides from α,ω -diiodoperfluoroalkanes. Regioselectivity of nucleophilic epoxide-ring opening and new amphiphilic compounds and monomers. *J. Fluorine Chem.* 102, 349-361 (2000).
5. Církva V., Böhm S., Paleta O.: Radical addition reactions of fluorinated species. Part 8. Regioselectivity of radical additions to perfluoroalkylethylenes and quantum chemical calculations. Highly selective two-step synthesis of 4-(perfluoroalkyl)butane-1,2-diols. *J. Fluorine Chem.* 102, 159-168 (2000).
6. Čermák Jan, Šabata S., Blechta V., Shaw B. L.: Nickel(0) and palladium(0) complexes with (Z,Z)- $\text{Ph}_2\text{PCH}_2\text{C}(\text{t-Bu})=\text{N}-\text{N}=\text{C}(\text{t-Bu})\text{CH}_2\text{PPh}_2$. Alkyne-to-alkenyl conversion in $[\text{Pd}(\text{MeOCOC}=\text{CCOOMe})\{(Z,Z)\text{-Ph}_2\text{PCH}_2\text{C}(\text{t-Bu})=\text{N}-\text{N}=\text{C}(\text{t-Bu})\text{CH}_2\text{PPh}_2\}]$. *Collect. Czech. Chem. Commun.* 65(1), 17-22 (2000).
7. Čermák Jan, Kvičalová M., Blechta V.: Pentamethylcyclopentadienylrhodium(I) complexes incorporated into porous polysiloxanes prepared by a sol-gel process: catalysts for hydrogenation of crotonic acid in water. *Appl. Organomet. Chem.* 14, 164-169 (2000).
8. Hájek M., Radoiu M.: Microwave activation of catalytic transformation of t-butylphenols. *J. Mol. Catal. A* 160, 383-392 (2000).
9. Šmíd J., Včelák J., Hanykýř V.: Messglied eines Gebers zur Ermittlung von Normal- und Tangentialspannungen in keramischen Massen, I. (Ger) Transmitter measuring

- element for the determination of normal and tangential tensions in ceramic compositions, I. *Keramische Z.* 52(6), 486-488 (2000).
10. Šmíd J., Včelák J., Hanykýř V.: Messglied eines Gebers zur Ermittlung von Normal- und Tangentialspannungen in keramischen Massen, II. (Ger) The transducer measuring element for the determination of normal and tangential stresses in ceramic compositions, II. *Keramische Z.* 52(7), 594-598 (2000).
 11. Vaňková R., Kuncová G.: Dvourozměrná fluorescenční spektroskopie - netradiční metoda pro stanovení viability rostlinných buněk. (Czech) Two-dimensional fluorescence spectroscopy - A new tool for plant cell viability estimation. *Biol. Listy* 65(3-4), 299-301 (in press).
 12. Vaňková R., Kuncová G., Sussenbeková H., Opatrná J.: Two-dimensional fluorescence spectroscopy - A new tool for plant cell viability estimation. *Plant Physiol. Biochem.* 38 (Suppl)15 (2000).
 13. Zimmerman H. E., Církva V.: The tri- π -methane rearrangement; mechanistic and exploratory organic photochemistry. *Org. Lett.* 2, 2365-2367 (2000).
 14. Czakoová M., Hetflejš J., Včelák J.: Substituent effects dehalogenation of aryl bromides with $\text{NaAlH}_2(\text{OCH}_2\text{OCH}_3)_2$. *React. Kinet. Catal. Lett.* (in press).
 15. Čermák Jan, Kvíčalová M., Šabata S., Blechta V., Vojtíšek P., Podlaha J., Shaw B. L.: Diphosphinoazines (Z,Z)- $\text{R}_2\text{PCH}_2\text{C}(\text{But})=\text{NN}=\text{C}(\text{But})\text{CH}_2\text{PR}_2$ with R groups of various sizes and complexes $[\{(Z,Z)\text{-R}_2\text{PCH}_2\text{C}(\text{But})=\text{NN}=\text{C}(\text{But})\text{CH}_2\text{PR}_2\} \{\eta^3\text{-CH}_2\text{C}(\text{CH}_3)=\text{CH}_2\}\text{PdCl}_2\}_2]$. *Inorg. Chim. Acta* (in press).
 16. Hájek M., Radoiu M. T.: Microwave induced reactions in liquid phase. *Ceram. Trans.* (in press).
 17. Hetflejš J., Czakoová M., Řeřicha R., Včelák J.: Catalyzed dehalogenation of Delor 103 by sodium hydridoaluminate. *Chemosphere* (in press).
 18. Kaštánek F., Demnerová K., Pazlarová J., Burkhard J., Maléterová Y.: Biodegradation of PCBs and VOC in soils and ground water. *Int. Biodeterior. Biodegrad.* (in press).
 19. Klán P., Hájek M., Církva V.: Photochemistry in a microwave oven. *J. Chem. Educ.* (in press).
 20. Škvára F., Kaštánek F., Pavelková I., Šolcová O., Maléterová Y., Schneider P.: Solidification of waste steel foundry dust with Portland cement. *J. Hazard. Mater.* (in press).
 21. Vaňková R., Kuncová G., Opatrná J., Sussenbeková H., Gaudinová A., Vaněk T.: Two-dimensional fluorescence spectroscopy - A new tool for determination of plant cell viability. *Plant Cell Rep.* (in press).
 22. Včelák J., Řeřicha R., Hetflejš J.: Metal complex-catalyzed dechlorination of chloroarenes by SDMA-side reactions. *Appl. Organometal. Chem.* (in press).
 23. Zimmerman H. E., Církva V.: The tri- π -methane rearrangement; excited and ground state versions: mechanistic and exploratory organic photochemistry. *J. Org. Chem.* (in press).

Review papers

24. Murová I., Hájek M., Lovás M.: Využitie mikrovlnnej energie pri chemickej úprave nerastných surovín. (Slov) Application of microwave energy to chemical treatment of mineral raw materials. *Chem. Listy* (in press).

Monographs

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Czech patents

26. Hájek M., Volf V., Vosáb J.: Způsob a zařízení ke zpracování sklářských materiálů. (Czech) Manufacture and equipment for glass material processing. Czech. Pat. PV 2185-99 (in press).
27. Hájek M.: Způsob a zařízení v tepelném zpracování sklářských materiálů. (Czech) Method and equipment for heat treatment of glass materials. Czech. Pat. PV 2000-968 (in press).
28. Hájek M., Drahoš J.: Způsob a zařízení k tepelnému zpracování přírodních materiálů, zvláště vulkanického původu. (Czech) Method and apparatus for heat treatment of glass materials and natural materials specifically of volcanic origin. Czech. Pat. PV 2000-1935 (in press).

International patents

29. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and apparatus for heat treatment of glass materials and natural materials specifically of volcanic origin. PCTI/CZ00/00042/ (in press).

Conferences

30. Čermák Jan, Auerová K., Nguyen H. T. T., Blechta V.: Rhodium complexes with cyclopentadienyl ligands containing perfluoroalkyl ponytails. 12th International Symposium on Homogeneous Catalysis ISHC 12, Book of Abstracts, p. 90, Stockholm University, Sweden, 27 August-1 September (2000).
31. Gruber V., Iwata H., Endoh S., Punčochář M., Drahoš J.: Some aspects of separation of gold(III) from multi-metallic solutions by n-butyl acetate extraction. International Workshop on Effective Utilization of Waste for Minimum Emission and its Safety, Proceedings, pp. 45-48, Kraków, Poland, 7-9 March (2000).
32. Hájek M.: Microwave activation of heterogeneous catalytic reactions in liquid phase. XXXIIInd Symposium on Catalysis, p. Op5, Prague, 6-7 November (2000).
33. Hájek M.: Microwave activation of catalytic reactions. International Conference on Microwave Chemistry, Proceedings, pp. 131-134, Antibes-Juan-les-Pins, France, 4-7 September (2000).
34. Hájek M.: Microwave heating of glass melts. NOVEM Workshop Energy Efficiency in Glass Production, pp. 94-97, Amsterdam, The Netherlands, 18-19 May (2000).
35. Hájek M.: Manufacture and processing of glass by microwave energy. 1st Slovak Glass Conference, Proceedings, pp. 33-34, Trenčín, Slovakia, 29 June-1 July (2000).
36. Hájek M., Církva V., Klán P.: Microwave photoreactor for photochemical synthesis. XVIIIth IUPAC Symposium on Photochemistry, Book of Abstracts, pp. 283-284, Dresden, Germany, 22-27 July (2000).
37. Hájek M., Radoiu M. T.: Microwave-induced catalytic reactions in liquid phase. 2nd World Congress on Microwave & Radio Frequency Processing, pp. 12-13, Orlando, Florida, USA, 2-6 April (2000).
38. Hájek M., Radoiu M. T., Kurfürstová J.: Microwave-induced catalytic reactions in liquid phase. 5th Pannonian International Symposium on Catalysis, Book of Abstracts, p. P-48, Kazimierz Dolny nad Wisla, Poland, 31 May-3 June (2000).
39. Kurfürstová J., Hájek M.: Microwave activation of catalytic reactions at low temperature. XXXIIInd Symposium on Catalysis, p. Po22, Prague, 6-7 November (2000).

40. Nebolová P., Nekvindová P., Perina V., Macková A., Jirka I., Kuncová G., Spirková J.: Copper containing glass for optical waveguides. 1st Balkan Conference on Glass Science & Technology, Proceedings, pp. 145-152, Volos, Grece, 9-10 October (2000).
41. Podešva J., Štěpánek P., Dybal J., Spěváček J., Hetflejš J.: Supramolecular structures in liquid polybutadienes. 38th Macromolecular IUPAC Symposium, Book of Abstracts, p. 1103, Warsaw, Poland, 9-14 July (2000).
42. Podrazký O., Klier D., Kuncová G., Karban J., Burkhard J., Pazlarová J., Demnerová K.: Biodegradation of polychlorinated biphenyls by immobilized *Pseudomonas species* 2. 12th Regional Central European Conference IUAPPA and 4th International Conference on Environmental Impact Assessment, Book of Abstracts, p. 97, Prague, Czech Republic, 11-14 September (2000).
43. Radoiu M. T., Kurfürstová J., Hájek M.: Catalytic transformation of t-butylphenols under microwave irradiation in the presence of montmorillonite KSF. International Conference on Microwave Chemistry, Proceedings, pp. 161-164, Antibes-Juan-les-Pins, France, 4-7 September (2000).
44. Szilva J., Kuncová G.: Immobilization of lipases by sol-gel method. 2nd International Conference on Protein Stabilisation/Biomolecule Stabilisation, posters P71, Lisbon, Portugal, 9-12 April (2000).
45. Škvára F., Kaštánek F., Pavelková I., Šolcová O., Maléterová Y., Schneider P.: Solidified waste steel foundry dust. 10th Symposium SILICHEM, Brno, Czech Republic, 22-23 June (2000).

Department of Reaction Engineering in Gas Phase

Head: M. Punčochář
Deputy: V. Ždímal

Research groups

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

Aerosol Laboratory

Research staff: J. Smolík, I. Ševčíková, J. Kugler, V. V. Levdansky, P. Moravec,
J. Schwarz, V. Ždímal
PhD students: D. Brus, L. Džumbová

Fields of research

- Particulate emissions from combustion processes
- Composition and size of atmospheric aerosols
- Synthesis of nanoparticles *via* aerosol processes
- Heat and mass transfer in aerosol systems
- Nucleation phenomena
- Interaction of aerosols with electromagnetic radiation

Research projects

Composition and mode of occurrence of the mineral constituents in brown coal and their behaviour during fluidised bed combustion

(J. Smolík, supported by GA ASCR, grant No. A2046904)

The project is aimed at study of composition and behaviour of minerals and inorganic elements during fluidised bed combustion in connection with their distribution and mode of occurrence. The information on modes of occurrence of elements in coal is obtained from selective leaching experiments. Special attention is also paid to the study of the effect of

mineral additives on the distribution of trace elements such as As, Cd, Hg, Ni, Pb, Se, V, and Zn in emitted particles. [Refs. 4, 17, 18, 20]

Reduction of heavy metal emissions from fluidised bed coal combustion using sorbents

(J. Schwarz, supported by GA CR, grant No. 104/00/1297)

The project represents both experimental and theoretical effort aimed at solving important relationships in the complex processes of combustion, formation of particulate emissions, and behaviour of metal pollutants within a fluidised bed and in flue gas cleaning units. The experimental part is focused on interaction of mineral sorbents with metallic species emitted from the fluidised bed combustion of coal. Theoretical part uses thermodynamic approach to predict distribution of trace elements into different emission streams. [Refs. 4, 17, 18, 20]

Gas phase synthesis of multicomponent nanoparticles

(P. Moravec, supported by GA ASCR, grant No. A4072807)

Project involves the synthesis of single-component fine particles and mixed and coated multicomponent nanoparticles by chemical vapour deposition in a tube reactor. Homogeneous particles of alumina and titania and/or coated mixed silica-alumina and titania-silica particles were prepared by decomposition of aluminum tri-*sec*-butoxide, titanium tetra-*iso*-propoxide and tetraethylortho-silicate. Particles were characterised by SEM, TEM and EDAX analysis. [Refs. 3, 7, 8, 15, 16]

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

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

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

Physicochemical properties of urban atmospheric aerosol. Source apportionment and impact on air quality

(J. Smolík, supported by AIE CR, grant No. KONTAKT 25)

In the project the urban atmospheric aerosols in Prague and Athens are studied. The aim is to identify the impact of various emission sources in the two cities and the prediction of the fate of key atmospheric aerosol species.

International co-operations

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

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

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

Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece: Urban aerosols
Norwegian Institute for Air Research, Kjeller, Norway: Formation of ozone and fine particles in the Mediterranean area
University of Essex, Colchester, U.K.: Sampling of fine atmospheric particles
Institute for Systems, Informatics and Safety, JRC-Ispra, Italy: Modelling of fine particle formation

Visits abroad

L. Džumbová: University of Helsinki, University of Tampere, Åbo University, Finland
J. Schwarz: University of Gent (RUG), Gent, Belgium (1 year)
J. Smolík: Research Centre "Demokritos", Athens, Greece and Meteorological station Finokalia, Crete, Greece (2 months), Eötvös University, Budapest, University of Veszprém, Veszprém, Hungary
V. Ždímal: Research Centre "Demokritos", Athens, Greece and Meteorological station Finokalia, Crete, Greece (2 months), Philipps-University, Marburg, Germany

Visitors

S. P. Bakanov, Institute of Physical Chemistry, Moscow, Russia
R. Heist, University of Rochester, Rochester, USA
M. Shapiro, Technion - Israel Institute of Technology, Haifa, Israel
Chuen-Jinn Tsai, National Chiao Tung University, Hsin Chu, Taiwan

Publications

Papers

1. Kim H. Y., Kim H. C., Levdansky V. V., Moravec P., Smolík J.: Protsessy perenosa v poristyxh katalizatorakh v pole mikrovolnovo izlucheniya. (Russ) Processes of transfer in pore catalysts in microwave field. *Inzh.-Fiz. Zh. (J. Eng. Phys.)* 73(4), 688-694 (2000).
2. Kim H. Y., Kim H. C., Levdansky V. V., Leitsina V. G., Smolík J.: Chemical deposition of substance from gas phase in nonisothermal channels. *Int. J. Heat Mass Transfer* 43, 3877-3882 (2000).
3. Levdansky V. V., Smolík J., Moravec P.: Trapping of impurity molecules in condensation from mixtures of gases. *Int. J. Heat Mass Transfer* 43(4), 629-637 (2000).
4. Smolík J., Schwarz J., Veselý V., Sýkorová I., Kučera J., Havránek V.: Influence of calcareous sorbents on particulate emissions from fluidized bed combustion of lignite. *Aerosol Sci. Technol.* 33, 544-556 (2000).

5. Bakanov S. P., Smolík J., Zaripov S. K., Ždímal V.: Continuum regime motion of a growing droplet in opposing thermo-diffusiophoretic and gravitational fields of a thermal diffusion cloud chamber. *J. Aerosol Sci.* (in press).
6. Bakanov S. P., Ždímal V., Zaripov S. K., Smolík J.: Matematicheskaya model' dvizheniya aerol'nykh chastits v termodiffuzionnoi kamere. (Russ) Mathematical model of motion of aerosol particles in a thermal diffusion cloud chamber. *Colloid. Zh.* (in press).
7. Levdansky V. V., Kim H. Y., Kim H. C., Smolík J., Moravec P.: Effect of electromagnetic fields on transfer processes in heterogeneous systems. *Int. J. Heat Mass Transfer* (in press).
8. Moravec P., Smolík J., Levdansky V. V.: Preparation of fine particles by decomposition of aluminum tri-sec-butoxide vapour. *J. Mater. Sci. Lett.* (in press).
9. Smolík J., Džumbová L., Schwarz J., Kulmala M.: Evaporation of ventilated water droplet: connections between heat and mass transfer. *J. Aerosol Sci.* (in press).

Conferences

10. Bakanov S. P., Ždímal V., Zaripov S. K., Smolík J.: Model' rastushchei kapli v termodiffuzionnoi kamere. (Russ) Model of droplet growth in a thermal diffusion cloud chamber. International Conference Honoring 90th Anniversary of G. G. Tumasheva, pp. 277-278, Kazan', Russia, 21-24 November (2000).
11. Kim H. I., Kim H. C., Levdansky V. V., Moravec P., Smolík J.: Effect of electromagnetic radiation on chemical reactions in heterogeneous systems. International Meeting on Chemical Engineering, Environmental Protection and Biotechnology AICHEM 2000, Abstracts of lecture groups Chemical Engineering and Reaction Technology, pp. 217-219, Frankfurt am Main, 22-27 May (2000).
12. Kim H. Y., Kim H. C., Levdansky V. V., Moravec P., Smolík J.: Vliyanie elektromagnitnogo izlucheniya na protsessy perenosa v dispersnykh sistemakh. (Russ) Influence of electromagnetic radiation on transfer processes in disperse systems. IV Minskii Mezhdunarodnyi Forum Teplomassoobmen MMF-2000, Tom 6, stp. 223-227, Minsk, 22-26 Maya (4th Minsk International Heat and Mass Transfer Forum MIF-2000, Abstracts, p. 101, Minsk, Republic of Belarus, 22-26 May) (2000).
13. Kim H. Y., Kim H. C., Levdansky V. V., Moravec P., Smolík J.: Chemical deposition in aerosol systems in field of electromagnetic radiation. *J. Aerosol Sci.* 31, S1, pp. S380-S381 (Abstract of the 2000 Europ. Aerosol. Conf., Dublin, 3-8 September) (2000).
14. Levdansky V. V., Smolík J., Moravec P.: Effect of growth rate of aerosol particles on impurity molecule trapping. V International School-Seminar Nonequilibrium Processes and Their Application, Contributed Papers, pp. 17-19, Minsk, Belarus, 1-6 September (2000).
15. Levdansky V. V., Smolík J., Moravec P.: Growth of small particles from gas mixtures. 19th European Conference on Surface Science ECOSS-19, Europhysics Conference Abstracts, Volume 24C, p. 153, Madrid, Spain, 5-8 September (2000).
16. Moravec P., Smolík J., Levdansky V. V.: Synthesis of titania particles by vapour-phase decomposition of titanium tetraisopropoxide. *J. Aerosol Sci.* 31, S1, pp. S927-S928 (Abstract of the 2000 Europ. Aerosol. Conf., Dublin, 3-8 September) (2000).
17. Smolík J., Schwarz J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate emissions from fluidised bed combustion of lignite with mineral sorbents. *J. Aerosol Sci.* 31, S1, pp. S670-S671 (Abstract of the 2000 Europ. Aerosol. Conf., Dublin, 3-8 September) (2000).

18. Smolík J., Schwarz J., Džumbová L., Kugler J., Veselý V.: Use of various sorbents for control of trace metal emissions from fluidised bed combustion of lignite. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 4, p. 269, Praha, 27-31 August (2000).
19. Stratmann F., Wilck M., Ždímal V., Smolík J.: First results of a new 2-D model for the description of thermal diffusion cloud chambers. *J. Aerosol Sci.* 31, S1, pp. S98-S99 (Abstract of the 2000 Europ. Aerosol. Conf., Dublin, 3-8 September) (2000).
20. Sýkorová I., Bouška V., Smolík J., Schwarz J., Džumbová L., Kučera J., Havránek V.: Solid emissions from the atmospheric fluidized-bed combustion of Czech lignite. 17th Annual Meeting of the Society for Organic Petrology, Book of Abstracts, pp. 91-93, Bloomington, Indiana, USA, 17-20 September (2000).
21. Ždímal V., Smolík J., Hopke P. K., Matas J.: Improvement of the homogeneous nucleation rate measurements in a static diffusion chamber with use of a CCD camera. 15th International Conference Nucleation and Atmospheric Aerosols 2000, Book of Abstracts, pp. 311-314, Rolla, USA, 6-11 August (2000).
22. Maenhaut W., Schwarz J., Cafmeyer J., Chi X.: Organic and elemental/black carbon during the EUROTRAC-2 AEROSOL Intercomparison-2000, 7th Int. Conf. on Carbonaceous Particles in the Atmosphere, San Juan, Puerto Rico, 26-29 November (2000)

Group of Hydrodynamics and Chemistry of Incineration

Research staff: M. Punčochář, E. Fišerová, V. Pekárek, V. Tydlitát

Technical staff: P. Hájek, J. Ullrich

PhD student: M. Jočová

Fields of research

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

Applied research

- Dechlorination of persistent organic pollutants
- Industrial and underground water treatment

Research projects

Power combustion of wastes and biomass

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

Experiments were done on the 100 kW CFB reactor with combustion of lignite, charcoal, and, as a source of chlorine, PVC powder was added in some experiments. The effect of sulfur compounds (diluted and concentrated sulfuric acid, sulfur dioxide with hydrogen peroxide) was explored for the reduction of polyhalogenated dibenzo-p-dioxins and benzofuran emissions. The most efficient additives for PCDD/F dropping, that we found, were the concentrated H_2SO_4 and the combination $\text{SO}_2 + \text{H}_2\text{O}_2$. The application of concentrated sulfuric acid depended strongly on the temperature in the place where the acid was applied. Big difference between application of diluted and concentrated acid were found in concentrations of PCDD on fly ash. The concentrated acid is much more efficient for removing of PCDD/F. We found that the different experience with influence of SO_2 in flue gas on PCDD/F formation is probably due to the equilibrium $\text{SO}_3 \leftrightarrow \text{SO}_2$. The strong correlation between concentration of dioxins and level of O_2 in flue gas was also experimentally proved. [Refs. 2, 7, 11]

Detoxification of polyhalogenated dibenzo-p-dioxins and benzofurans on catalytically active surfaces of inorganic sorbents

(V. Pekárek, supported by GA ASCR, grant No. A4072901)

The fly ashes from municipal waste incinerators contain significant amounts of persistent organic pollutants from which the dioxins and benzofurans are of the highest chemical stability and toxicity. Their detoxification by means of dehalogenation on catalytically active surfaces was therefore studied. It was found that the dehalogenation efficiency of ash depends on the quality of skeleton, presence of metals, amount and chemical form of carbon and on the reaction conditions. A synthetic analogue of ash was created for optimal dehalogenation. Using this synthetic ash, HCB was totally converted to the benzene and Delor 103 to biphenyl. A mixed batch reactor was built for dehalogenation of PCB in waste oil. Further, experiments were done for explanation of SO_2 , H_2O_2 and H_2SO_4 influence on the course of novosynthetic reactions in the system extracted ash, $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$, and NaCl at 340 °C. [Refs. 2, 4, 7]

Cleaning of underground water by coal based sorbents

(M. Punčochář, supported by Grant Agency of Ministry of Environment, grant No. VaV 550/1/99)

Calcium loaded coal is used for removing heavy metals and organic pollutants from underground water. Lignite loaded by calcium is an effective ion-exchanger. Coal with metal and organic pollutants is combusted in a fluidized bed with simultaneous capture of fly ash and flue gas pollutants. A model was developed for prediction of ion exchange in coal. [Ref. 9]

International co-operation

NIRE, Tsukuba, Japan: Resources recycling in Eastern Europe

Visits abroad

M. Punčochář: Japan Tokyo University, Hokkaido University, NIRE, Tsukuba, Japan (1 month)

Visitors

H. Iwata: NIRE, Tsukuba, Japan

Publications

Papers

1. Brož J., Grabic R., Kilián J., Lojkásek M., Marklund S., Ocelka T., Pekárek V., Příbyl J., Tydlitát V., Výška J.: The effect of oils on PAH, PCDD, PCDF, and PCB emissions from a spark engine fueled with leaded gasoline. *Chemosphere* 41, 1905-1911 (2000).
2. Grabic R., Pekárek V., Ulrich J.: Effect of reaction time on formation of PCB, PCDD and PCDF in the system containing extracted fly ash, copper chloride, activated carbon, oxygen and nitrogen atmosphere. *Organohalogen Compd.* 46, 209-212 (2000).
3. Punčochář M., Drahoš J.: Limits of applicability of capillary model for pressure drop correlation. *Chem. Eng. Sci.* 55(18), 3951-3954 (2000).
4. Stach J., Pekárek V., Grabic R., Lojkásek M., Pacáková V.: Dechlorination of polychlorinated biphenyls, dibenzo-p-dioxins and dibenzofurans on fly ash. *Chemosphere* 41, 1881-1887 (2000).
5. Tydlitát V., Pekárek V., Marklund S., Grabic R.: Persistentní organické látky v motorových emisích při použití olovnatého benzínu a různých olejů. (Czech) Persistent organic pollutants in emissions of a spark engine fed with leaded gasoline with the use of different oils. *Ochrana ovzduší* 6, 4-7 (2000).
6. Vrba J., Punčochář M., Drahoš J.: Fuzzy decomposition applied on logistic equation. *SAMS* 38, 65-80 (2000).
7. Pekárek V., Marklund S., Grabic R., Punčochář M., Ulrich J.: Effects of oxygen on formation of polychlorinated biphenyls (PCB), dibenzo-p-dioxins (PCDD) and dibenzofurans (PCDF) on the extracted municipal waste incinerator fly ash in the presence of carbon and cupric salt. *Chemosphere* (in press).

Conferences

8. Gruber V., Iwata H., Endoh S., Punčochář M., Drahoš J.: Some aspects of separation of gold(III) from multi-metallic solutions by n-butyl acetate extraction. *International Workshop on Effective Utilization of Waste for Minimum Emission and its Safety, Proceedings*, pp. 45-48, Kraków, Poland, 7-9 March (2000).
9. Jochová M., Horáček J., Punčochář M., Drahoš J.: Recovery of heavy metals from waste water. *International Workshop on Effective Utilization of Waste for Minimum Emission and its Safety, Proceedings*, pp. 87-93, Kraków, Poland, 7-9 March (2000).

10. Pekárek V.: Importance of reprocessing of the fly ash from municipal waste and hazardous waste incinerators. Workshop on Control Options/Technologies to Abate Heavy Metal and Persistent Organic Pollutant Emissions from Stationary Sources and Products, Proceedings, pp. 51-55, Průhonice, Czech Republik, 26-28 April (2000).
11. Punčochář M., Veselý V., Grabic R., Tydlitát V., Pekárek V.: The influence of water, sulfur and hydrogen peroxide on PCD/F formation. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 4, p. 292, Praha, 27-31 August (2000).

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

Research staff: M. Hartman, Ji. Čermák, K. Svoboda, O. Trnka, V. Veselý

Technical staff: J. Chour, 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

Applied research

- Know-how for the combustion of waste organic materials in fluidized bed [Ref. 8]

Research projects

Reaction and reactors for hot coal-gas desulphurization with calcareous materials

(M. Hartman, supported by GA ASCR, grant No. A4072711)

Possibilities of using various calcareous materials are explored for hot coal-gas desulphurization. Practical reaction rate equations are developed and incorporated into tractable models of the reactors for contacting coal-gas with solid sorbents. [Refs. 1, 2, 4, 14]

Important reactions in the fluidized bed

(M. Hartman, supported by GA CR, grant No. 203/98/0101)

Kinetics of the thermal dehydration of inorganic hydrates are explored. Particular attention is given to the softening, agglomeration and possible defluidization of particles caused by chemical reactions. [Refs. 5, 6, 7]

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

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

The project in the field of Clean Coal Technology and biomass-co-combustion is concentrated on experimental investigation and modelling of pressurized bed combustion of coal and biomass-coal blends. Target of the research work: emissions (NO_x , N_2O , CO , SO_2), maximum particle temperature and agglomeration of coal/biomass-ash particles. [Refs. 1, 9-13, 22]

Low emissions with extremely staged (pressurized) coal combustion - A novel concept

(K. Svoboda, supported by the EC in the program INCO-Copernicus, Contract No. ERBIC15-CT98-0513)

The project, with experimental and theoretical part, is focused on differences between oxidizing, slightly reducing and air staging conditions in pressurized fluidized bed combustion of selected coals on overall emissions, (esp. NO , N_2O , SO_x) in modern coal combined cycle power generation. [Refs. 2, 11-13, 15, 16, 20-22]

International co-operations

University College London, London, UK: Settling of non-spherical particles

University of Connecticut, Storrs, USA: Reactivity of solids

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

Technical University Cottbus, Germany: Pressurized fluidized bed combustion

Institute of Physical Chemistry, PAS, Warsaw, Poland: Special regimes of fluidization

DMT Essen, Germany: Pressurized fluidized bed combustion

Visits abroad

M. Hartman: ACHEMA, Frankfurt/M, Germany

K. Svoboda: Institute of Chemical Metallurgy Academia Sinica, Beijing, China

K. Svoboda: Chalmers Univ. of Technology, Göteborg, Sweden

Visitors

D. Ziolkowski: Institute of Physical Chemistry, PAS, Warsaw, Poland

J. Michalski: Institute of Physical Chemistry, PAS, Warsaw, Poland

H. J. Krautz: BTU Cottbus, Germany

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

Teaching

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

K. Svoboda: ICT, course "Environmental protection"

Publications

Papers

1. Hartman M., Trnka O., Svoboda K.: Fluidization characteristics of dolomite and calcined dolomite particles. *Chem. Eng. Sci.* 55(24), 6269-6274 (2000).
2. Hartman M., Trnka O., Svoboda K.: Essential factors in removing carbonyl sulphide from coal gas with lime and limestone. *Chem. Papers* 54(5), 302-306 (2000).
3. Smolík J., Schwarz J., Veselý V., Sýkorová I., Kučera J., Havránek V.: Influence of calcareous sorbents on particulate emissions from fluidized bed combustion of lignite. *Aerosol Sci. Technol.* 33, 544-556 (2000).
4. Trnka O., Veselý V., Hartman M., Beran Z.: Identification of the state of a fluidized bed by pressure fluctuations. *AIChE J.* 46(3), 509-514 (2000).
5. Hartman M., Trnka O., Veselý V., Svoboda K.: Thermal dehydration of the sodium carbonate hydrates. *Chem. Eng. Commun.* (in press).
6. Hartman M., Veselý V., Svoboda K., Trnka O., Beran Z.: Dehydration of sodium carbonate decahydrate to monohydrate in a fluidized bed. *AIChE J.* (in press).
7. Hartman M., Trnka O., Veselý V., Svoboda K.: Properties of sodium carbonate's beds at incipient fluidization and terminal velocities of solids. *Chem. Pap.* (in press).
8. Veselý V., Hartman M., Svoboda K., Trnka O.: Spalování kapalných paliv ve fluidní vrstvě. (Czech) Incineration of liquid wastes in fluidized bed. *Chem. Listy* (in press).

Review papers

9. Svoboda K., Čermák Ji.: Chemistry and emissions of nitrogen oxides (NO, NO₂, N₂O) in combustion of solid fuels. I. Heterogeneous reactions - NO + NO₂. *Chem. Pap.* 54(2), 104-117 (2000).
10. Svoboda K., Čermák Ji., Hartman M.: Chemistry and emissions of nitrogen oxides (NO, NO₂, N₂O) in combustion of solid fuels. II. Heterogeneous reactions - N₂O. *Chem. Pap.* 54(2), 118-130 (2000).

Monographs

11. Svoboda K., Hartman M., Čermák Ji.: Combustion mechanisms - solid phase: Structural changes and heterogeneous reactions. *Pollutants from Combustion*, C. Vovelle (ed.), pp. 35-50, Kluwer Academic Publishers (2000).
12. Svoboda K., Hartman M., Čermák Ji.: NO_x chemistry and emissions - I: Heterogeneous reactions (NO + NO₂). *Pollutants from Combustion*, C. Vovelle (ed.), pp. 145-163, Kluwer Academic Publishers (2000).
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Czech patents

14. Veselý V., Trnka O., Hartman M.: Způsob řízení a identifikace režimů fluidující vrstvy zrnitého materiálu. (Czech) Control and identification of a regime of the fluidized bed. Czech. Pat. (in press).

Conferences

15. Čermák Ji., Svoboda K., Pohořelý M.: Zkušenosti s užitím FT-IR analyzátoru pro analýzu spalin. (Czech) Our experiences with FT-IR analyzer in the field of flue and off gas measurement. 27th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 115, Tatranské Matliare, Slovakia, 22-26 May (2000).
16. Čermák Ji., Svoboda K., Pohořelý M.: Application of FT-IR analyzers in measurements of flue and exhaust gas components. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 4, p. 286, Praha, 27-31 August (2000).
17. Punčochář M., Veselý V., Grabic R., Tydlitát V., Pekárek V.: The influence of water, sulfur and hydrogen peroxide on PCD/F formation. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 4, p. 292, Praha, 27-31 August (2000).
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19. Smolík J., Schwarz J., Džumbová L., Kugler J., Veselý V.: Use of various sorbents for control of trace metal emissions from fluidised bed combustion of lignite. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 4, p. 269, Praha, 27-31 August (2000).
20. Svoboda K., Klika Z., Čermák Ji., Hartman M., Pohořelý M.: Substoichiometric combustion of coals, emissions of sulfur and nitrogen compounds. Technical Progress Meeting, Levice, Slovakia, 17 February (2000).
21. Svoboda K., Čermák Ji., Hartman M., Klika Z.: Influence of coal and operating conditions on performance and sulfur removal in advanced, staged PFBC. 14th International Congress of Chemical and Process Engineering CHISA 2000, Summaries 4, p. 287, Praha, 27-31 August (2000).
22. Svoboda K., Čermák Ji., Hartman M., Pohořelý M.: Possible ways of suppression of agglomeration of particles in fluidized bed combustion of selected waste biomass. Energy Forum 2000, Program, p. 115, Varna, Bulgaria, 17-19 September (2000).

Laser Chemistry Group

Research staff: J. Polá, V. Dřínek, R. Fajgar, A. Galík, A. Galíková, J. Kupčík, D. Pokorná,
M. Urbanová
Part time: K. Vacek
PhD student: K. Jursíková

Fields of research

- IR laser induced chemistry
- IR and UV laser induced chemical vapour deposition of novel polymeric and Si-based materials
- UV laser-induced polymerization in the gas phase
- UV laser-induced photolysis of organosilicon, organoselenium and organotellurium compounds
- IT laser ablative deposition of silicon monoxide and polymeric films

Research projects

Laser induced decomposition of hydridodisiloxanes

(J. Pola, supported by GA ASCR, grant No. A4072806)

IR laser induced gas-phase and liquid-phase decompositions of various polyhydridodisiloxanes have been studied to reveal suitability of these reactions for production of novel silicon-based materials. The examination of CO₂ laser-induced graphite-photosensitized decomposition of hydridomethylphenyldisiloxanes was shown to take place via silanone extrusion and afford a blend of poly(phenylsiloxanes) [Ref. 23]. IR laser induced homogeneous decomposition of gaseous hydridoalkyldisiloxanes is dominated by elimination and polymerization of transient silanones. This process represents a convenient chemical vapour deposition of poly(hydridoalkylsiloxane) films [Refs. 3, 7, 8, 20, 21, 25]. UV laser photolysis of hydridomethylsiloxanes is controlled by dehydrogenation and yields nano-textured hydrogenated Si/O and Si/C/O phases [Refs. 15, 17, 21, 26].

Laser induced synthesis of novel polymers

(J. Pola, supported by Ministry of Education, grant No. ME192)

ArF and N₂ laser photolysis of gaseous unsaturated organyltrimethylsilanes allows a unique photopolymerization in the absence of photo-initiators, which is suitable for chemical vapour deposition of solid poly(trimethylsilylhydrocarbon), poly(trimethylsilyloxyhydrocarbon) and polysiloxane films [Refs. 4, 5, 13, 18, 24]. The materials and the process are promising for biomedical applications and coating industry.

Improvement of organic photochemical reaction control by using lasers

(J. Pola, supported by Ministry of Education, grant No. ME191)

ArF and KrF laser photolytic cleavage of selenophene and tellurophene yields elemental Se and Te together with products of 1,3-H shift and β -C-C cleavage of the postulated C₄H₄ diradical intermediate. The relative importance of both channels is affected by the photon energy and the heteroatom. The process is promising for chemical vapour deposition of selenium and tellurium films [Refs. 6, 9]. KrF laser photolysis of gaseous dialkyl selenium and tellurium compounds results in efficient chemical vapour deposition of Se films and nano-structured Te powders [Refs. 11, 14].

IR laser-induced photochemistry of polysilanes for chemical vapour deposition of Si/C/H phases

(J. Pola, supported by Ministry of Education, grant No. ME392)

IR laser photolysis of 1,1,1,3,3,3-hexamethyl-2,2-divinyl-trisilane and IR laser ablation and UV laser photolysis of dodecamethylcyclohexasilane has been examined to show behaviour of these polysilanes under intense laser light.

Laser photochemistry of (chloromethyl)silane and silacyclopent-3-ene for chemical vapour deposition of Si/C/H and Si/H phases

(J. Pola, supported by GA CR, grant No. 104/00/1294)

IR laser thermolysis of silacyclopent-3-ene results in extrusion of silylene and can serve as efficient method for chemical vapour deposition of polycarbosilane films produced via reactions of silylene, butadiene and methylene [Ref. 10]. IR laser powered homogeneous decomposition of gaseous (chloromethyl)trimethylsilane is controlled by 1,2-Cl shift and extrusion of carbene [Ref. 19].

Laser ablation and chemistry of silicon monoxide

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

IR laser ablation of silicon monoxide in the absence and presence of gaseous water, hydrogen, carbon monoxide and methanol has been studied to explore reactivity of ablated particles towards these compounds. The films obtained via reactions of silicon monoxide with the above molecules were characterized by FTIR and XP spectroscopy and electron microscopy.

Laser induced decomposition of hydridosiloxanes

(J. Pola, supported by Ministry of Education)

IR laser decomposition of hydridosiloxanes under conditions of dielectric breakdown [Ref. 3] and reactions of hydridosiloxanes with Cl atoms has been studied. The results show that the reactivity of the Si-H bond in disiloxanes towards Cl is higher than that of the C-H bond. Both systems afford polymeric deposits, which were characterized by spectral methods and electron microscopy.

International co-operations

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

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

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

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

Institute of Spectroscopy, RAS, Troitsk, Russia: IR photolysis of silacycles in the condensed state

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

Technical University, Graz, Austria: Laser chemistry of polysilanes

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

Visits abroad

K. Jursíková: CEA-Saclay-DRECAM, France (1 month)

J. Kupčák: Institute of Materials and Chemical Research, Tsukuba, Japan (1.5 months)
J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (3 months)

Visitors

A. Ouchi: Institute of Materials and Chemical Research, Tsukuba, Japan
M. Santos: Instituto de Estructura de la Materia, CSIC Madrid, Spain
W. Stanczyk: Centre of Molecular and Macromolecular Studies, PAS, Lodz, Poland
A. Yabe: Institute of Materials and Chemical Research, Tsukuba, Japan

Publications

Papers

1. Fajgar R., Pola J.: Trimethylsilyl group migration in Criegee intermediate in gas-phase ozonolysis of trimethylsilylethene. *Tetrahedron Lett.* 41, 2435-2438 (2000).
2. Galíková A., Galík A.: Gravimetric study of the dynamics of adsorption and desorption of ammonia on γ -alumina. *Chem. Pap.* 54(4), 210-214 (2000).
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5. Pola J., Urbanová M., Bastl Z., Šubrt Z., Sakuragi M., Ouchi A., Morita H.: Laser-induced formation of polymers from unsaturated (organyl)trimethylsilanes in the gas phase. *Polymer* 42(4), 1311-1318 (2000).
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11. Pola J., Bastl Z., Šubrt J., Ouchi A.: Atmospheric pressure chemical vapour deposition of selenium films by KrF laser photolysis of dimethylselenium. *Appl. Surf. Sci.* 6713, 1-5 (2000).
12. Fajgar R., Pola J.: Trimethylsilyl group migrations in cryogenic ozonolysis of trimethylsilylethene: evidence for non-concerted primary ozonide decomposition pathway. *Chem.-Eur. J.* (in press).
13. Morita H., Ono H., Bastl Z., Pola J.: Laser-induced thin film formation from gaseous mixture of trimethylsilylacetylene and methyl acrylate. *J. Photochem. Photobiol., A* (in press).
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17. Pola J., Galíková A., Galík A., Bastl Z., Šubrt J., Ouchi A., Sakuragi M.: UV laser photolysis of disiloxanes for chemical vapour deposition of nano-textured silicones. *Chem. Mater.* (in press).
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19. Urbanová M., Pola J.: IR laser-powered homogeneous decomposition of (chloromethyl)-trimethylsilane: 1, 2-Cl shift and methene expulsion yielding chlorotrimethylsilane. *J. Anal. Appl. Pyrolysis* (in press).
20. Urbanová M., Bastl Z., Šubrt J., Pola J.: IR laser-induced thermolysis and UV laser-induced photolysis of 1, 3-diethyldisiloxane for chemical vapour deposition of nano-textured hydridoalkylsilicones. *J. Mater. Chem.* (in press).

Review papers

21. Pola J.: Laser gas-phase photolysis of organosilicon compounds: approach to formation of hydrogenated Si/C, Si/C/F, Si/C/O and Si/O phases. *Review Journal PINSA A(Physical Sciences)* 66, 107-136 (2000).

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24. Morita H., Semba K., Pola J.: Photochemical reactivity of trimethylsilylacetylene in UV laser-induced aerosol particle formation with acrolein. 3rd International Symposium on Photoreaction Control and Photofunctional Materials, Book of Abstracts, pp. 178-179, Tsukuba, 15-17 March (2000).

25. Pola J., Urbanová M., Galík A., Galíková A., Bastl Z., Šubrt J., Beckers H., Papagiannakopoulos P.: IR laser-induced decomposition of hydridosiloxanes for chemical vapour deposition of nanostructured hydridosilicone phases. 3rd NIMC International Symposium on Photoreaction Control and Photofunctional Materials, Book of Abstracts, pp. 174-175, Tsukuba, 15-17 March (2000).
26. Pola J., Urbanová M., Galíková A., Galík A., Bastl Z., Šubrt J., Ouchi A., Papagiannakopoulos P., Beckers H.: Laser photo-deposition of nano-textured poly(hydridosiloxanes) from gaseous disiloxanes. 3rd SANKEN International Symposium on Advanced Nanoelectronics: Devices, Materials, and Computing, Proceedings, pp. 205-206, Osaka University, 14-15 March (Vol. 57, Special Issue of Memoirs of the Institute of Scientific and Industrial Research) (2000).

Department of Analytical Chemistry

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

Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

Applied research

- Analytical services to the research departments of ICPF

Research projects

²⁹Si NMR chemical shifts

(J. Schraml, supported by GA CR, grant No. 203/99/0132)

A continued study of electronic and steric effects on the NMR chemical shifts of ²⁹Si and their utilization in the analysis of complex systems. [Refs. 12, 14]

VNMR NET

(J. Schraml, supported by Ministry of Education of Czech Republic, project LB98233)

Creation of a network of NMR laboratories within the country on the basis of a united hardware platform and software means.

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

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

Spectral studies of derivatives of hydroxamic acids under different experimental conditions and states of matter with the aim to determine the dependence of their structure on the environmental conditions. [Refs. 7-9, 13, 21]

International co-operations

University of Ghent, Ghent, Belgium: Study of Neurotoxins as Food Contaminants

Catholic University of Leuven, Leuven, Belgium: NMR in medicinal chemistry
Institute of Organic Chemistry, BAS, Sofia, Bulgaria: Dynamic NMR

Visits abroad

J. Schraml: Catholic University of Leuven, Leuven, Belgium

Teaching

J. Schraml: CU, course "NMR Spectroscopy"

Publications

Papers

1. Balcar H., Kubát P., Pacovská M., Blechta V.: Polyacetylene with coumarin containing pendant groups by polymerization of 7-propargyloxy-4-methylcoumarin. *Polym J. (Tokyo)* 32 (4), 370-374 (2000).
2. Balcar H., Čejka J., Kubišta J., Petrusová L., Kubát P., Blechta V.: Preparation and properties of isomeric N-(4-substituted benzylidene)-4-ethynylanilines and 4-substituted N-(4-ethynylbenzylidene)anilines. *Collect. Czech. Chem. Commun.* 65(2), 203-215 (2000).
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6. Lescrinier E., Esnouf R., Schraml J., Busson R., Heus Ha., Hilbers C. W., Herdewijn P.: Solution structure of a HNA-RNA hybrid. *Chem. Biol.* 7(9), 719-731 (2000).
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8. Schraml J.: Derivatives of hydroxamic acids. *Appl. Organometal. Chem.* 14, 604-610 (2000).
9. Schraml J., Kvičalová M., Blechta V., Soukupová L., Exner O., Boldhaus H.-M., Erdt F., Bliefert C.: Structure determination of dihydroxamic acids and their trimethylsilyl derivatives by NMR spectroscopy. *Magn. Reson. Chem.* 38, 795-801 (2000).

10. Čermák Jan, Kvičalová M., Šabata S., Blechta V., Vojtíšek P., Podlaha J., Shaw B. L.: Diphosphinoazines (Z, Z)-R₂PCH₂C(But)=NN=C(But)CH₂PR₂ with R groups of various sizes and complexes [$\{(Z, Z)\text{-R}_2\text{PCH}_2\text{C(But)=NN=C(But)CH}_2\text{PR}_2\}\{\eta^3\text{-CH}_2\text{C(CH}_3\text{)=CH}_2\}\text{PdCl}_2$]. *Inorg. Chim. Acta* (in press).
11. Hetflejš J., Czakoová M., Řeřicha R., Včelák J.: Catalyzed dehalogenation of Delor 103 by sodium hydridoaluminate. *Chemosphere* (in press).
12. Osson A., De Bruyn A., Schraml J., Herdewijn P., De Keukeleire D.: A novel polyhydroxylated alkaloidal amine from *Solanum elaeagnifolium* with β -glucosidase- and neuraminidase inhibiting activity. *FEBS Lett.* (in press).
13. Podlaha J., Císařová I., Kvičalová M., Schraml J.: Self-assembly of 4-nitrobenzhydroxamic acid in the crystal. *Supramol. Chem.* (in press).
14. Schraml J., Blechta V., Soukupová L., Petráková E.: DOSY of silylated saccharides. *J. Carbohydr. Chem.* (in press).
15. Včelák J., Řeřicha R., Hetflejš J.: Metal complex-catalyzed dechlorination of chloroarenes by SDMA-side reactions. *Appl. Organometal. Chem.* (in press).

Conferences

16. Balcar H., Sedláček J., Zedník J., Vohlídal J., Blechta V.: Polymerization of unconventional monosubstituted acetylenes with metathesis and insertion catalysts. XXXII Ind Symposium on Catalysis, p. Op8, Prague, 6-7 November (2000).
17. Čermák Jan, Auerová K., Nguyen H. T. T., Blechta V.: Rhodium complexes with cyclopentadienyl ligands containing perfluoroalkyl ponytails. 12th International Symposium on Homogeneous Catalysis ISHC 12, Book of Abstracts, p. 90, Stockholm University, Sweden, 27 August-1 September (2000).
18. Jochová M., Horáček J., Punčochář M., Drahoš J.: Recovery of heavy metals from waste water. International Workshop on Effective Utilization of Waste for Minimum Emission and its Safety, Proceedings, pp. 87-93, Kraków, Poland, 7-9 March (2000).
19. Lescrinier E., Schraml J., Busson R., Herdewijn P.: Solution structure of a hexitol nucleic acid duplex with four consecutive T: T base pairs. 4. Iglar NMR Tage, p. P8, Innsbruck, 10-11 February (2000).
20. Podrazký O., Klier D., Kuncová G., Karban J., Burkhard J., Pazlarová J., Demnerová K.: Biodegradation of polychlorinated biphenyls by immobilized *Pseudomonas species* 2. 12th Regional Central European Conference IUAPPA and 4th International Conference on Environmental Impact Assessment Prague 2000, Book of Abstracts, p. 97, Prague, Czech Republic, 11-14 September (2000).
21. Schraml J.: NMR studies of hydroxamic acids and their derivatives. 22nd Discussion Meeting Progress in the Magnetic Resonance of Bioactive Compounds and New Materials, Book of Abstracts, p. 48, Regensburg, Germany, 27-30 September (2000).

Miscellaneous

International Advisory Board of ICPF

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Organization of International Conferences and Scientific Meetings

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CHISA 2000 - 14th International Congress of Chemical and Process Engineering, Praha, 27–31 August

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