

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 1999

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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 18)
- Department of Multiphase Reactors (page 24)
- Department of Biotechnology and Environmental Processes (page 30)
- Department of Reaction Engineering in Gas Phase (page 37)
- Department of Analytical Chemistry (page 48)

STAFF
(31 December 1999)

Category	Number of Employees
Research □	108 □
Technical □	27 □
Administrative □	15 □
Services □	14 □

BUDGET 1999
(in million Kč; 35 Kč = 1 US\$, approx.)

Institutional support from National Budget	46
Research funds from Grant Agencies	27
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
PICT	Institute of Chemical Technology, Prague
CTU	Czech Technical University, Prague
CU	Charles University, Prague
TU	Technical University

Department of Diffusion and Separation Processes

Head: K. Jeřábek
Deputy: A. Heyberger
Research staff: L. Hanková, V. Jiříčný, J. Procházka, Z. Prokop, J. Roček, H. Sovová,
P. Uchytíl, 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, J. Vachtová, P. Veverka

Fields of research

- Transport properties of polymer and ceramic membranes, preparation of ceramic membranes
- 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 hydroxycarboxylic acids; extraction and refining of phenols from coal tars; liquid-liquid extraction of heavy metals; determination of organic pollutants in water
- 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 phenols from tars
- Extraction refining of digitalis plant alkaloids
- Refining of plant extracts
- Preparation of corundum support for ceramic membranes
- Analysis of function of the catalytic reactor for bisphenol A synthesis

Research projects

Composite ceramic membranes

(J. Roček, supported by GA CR, grant No. 104/97/1216)

Ceramic microfiltration membranes with narrow pore size distribution and good mechanical properties were prepared. Mathematical model of the gas permeation was used for

the study of the influence of the transport direction on the gas permeation in asymmetric ceramic membranes [Ref. 17].

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 [Ref. 29].

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 the accessibility of metal nanoparticles inside the gel polymer matrix [Ref. 9].

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. 10].

Regime of packed column as equipment with trickle-bed and bubble-bed in series

(V. Staněk, supported by GA CR, grant No. 203/97/1174)

Experimental apparatus for simultaneous measurement of hydrodynamic variables as a liquid hold up, pressure drop profiles, RTD in gas and liquid phase has been developed. The pressure and liquid hold up overshoot following sudden increase of gas or liquid flow have been observed and described by a mathematical model. Extensive 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. 6, 16, 24, 25, 27]

Effect of acid structure and solvent composition in extraction of organic acids by tertiary amines

A. Heyberger, supported by GA CR, grant No. 104/97/1213)

Equilibria in systems aqueous solution of tartaric and succinic acids - solution of trioctylamine in the mixture of inert diluent and polar modifier were measured, and a model describing the effect of diluents and their binary mixtures was formulated. [Refs. 3, 4, 7, 14]

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. [Refs. 18, 28]. Extraction of tungsten from aqueous solutions of sodium tungstate with solutions of trialkylamine in mixtures of tributyl phosphate in kerosene was investigated. Before extraction the organic phase was presaturated with sulphuric acid. Measurements at various values of constant pH were compared.

Solubilities in supercritical fluids - measurement and modelling

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

In connection with supercritical fluid extraction of natural products, high-pressure phase equilibria in the ternary system limonene + vegetable oil + CO₂ and in the corresponding binary systems with CO₂ [Ref. 15] were studied, and solubility of β -carotene in oil-saturated CO₂ was measured. Supercritical fluid extraction of peppermint oil was studied and compared with hydrodistillation [Ref. 1].

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 Inst. Org. Chem. Biochem. and PICT, supported by GA CR, grant No. 203/99/1457)

Enzymatic reactions of black currant oil were performed in water-saturated supercritical carbon dioxide using various arrangements. Best results were obtained with continuous flow of the reaction mixture through fixed bed of immobilised enzyme.

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

Weizmann Institute of Science, Rehovot, Israel: Polymer supported ligands

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

Visits abroad

A. Heyberger: University of Durban, AECL, South Africa

A. Heyberger: University of Linz, Austria

K. Jeřábek: Universities of Padua and L'Aquila, Italy

K. Jeřábek: Rohm and Haas, Spring House, USA

J. Procházka: University of Skopje, Macedonia

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

Visitors

A. D'Archivio, B. Corain, University of L'Aquila, Italy
A. Biffis, M. Zecca, University of Padua, Italy
P. Jonsson, Royal Institute of Technology, Stockholm, Sweden
I. Mishonov, Institute of Chemical Engineering, Sofia, Bulgaria
R.P. Stateva, Institute of Chemical Engineering, Sofia, Bulgaria
R. Tomovska, University of Skopje, Macedonia

Teaching

K. Jeřábek: PICT, postgraduate course "Fundamentals of preparation of heterogeneous catalysts"

Publications

Papers

1. Aleksovski S., Sovová H., Poposka F. A., Kulevanova S., Ristič M.: Comparison of essential oils obtained from *Mentha piperita* L. using supercritical carbon dioxide extraction and hydrodistillation. *Acta Pharm.* 49(1), 51-57 (1999).
2. Katz S., Staněk V., Landefeld C., Bauer M. E.: The AFS cupola process model: A computer tool for foundries. *Mod. Casting*, June, pp. 41-43 (1999).
3. Mishonov I., Procházka J., Heyberger A.: Extraction of D-tartaric acid with Alamine 336/LIX 54 mixture. *Collect. Czech. Chem. Commun.* 64(12), 2061-2072 (1999).
4. Poposka F., Procházka J., Tomovska R., Nikolovski K., Grizo A.: Extraction of tartaric acid from aqueous solutions with triisooctylamine (HOSTAREX A 324). Equilibrium and kinetics. *Chem. Eng. Sci.* 55(9), 1591-1604 (2000).
5. Sovová H., Rat V., Khachaturjan M., Vlček D.: Solubility of squalane and dinonyl phthalate in CO₂ with entrainers. *J. Supercrit. Fluids* 14(2), 145-149 (1999).
6. Staněk V., Jakeš B., Ondráček J., Jiříčný V.: Characteristics of pressure and liquid holdup overshoot following a sudden increase of gas flow. *Chem. Biochem. Eng. Q.* 13(2), 65-71 (1999).
7. Tomovska R., Poposka F., Heyberger A., Procházka J.: pH dependence of tartaric acid extraction. *Chem. Biochem. Eng. Q.* 13(4), 158-190 (1999).
8. Veverka L., Jeřábek K.: Mechanism of hypercrosslinking of chloromethylated S-DVB copolymers. *React. Func. Polym.* 41(1-3), 21-25 (1999).
9. 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.* (in press).
10. 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.* (in press).
11. Howdle S. M., Jeřábek K., Leocorbo V., Marr P. C., Sherrington D. C.: Reversibly collapsible macroporous poly(styrene-divinylbenzene) resins. *Polym. Commun.* (in press).

12. 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.* (in press).
13. Jiříčný V., Roy A., Evans J. W.: Electrodeposition of zinc from sodium zincate/hydroxide electrolytes in a spouted bed electrode. *Metall. Mater. Trans.* (in press).
14. Poposka F. A., Procházka J., Nikolovski K., Tomovska R.: Extraction of tartaric acid from aqueous solutions with triisooctylamine (HOSTAREX A 324). Simulation on the process in a reciprocating-plate extraction column. *Bull. Chem. Technol. Macedonia* (in press).
15. Sovová H.: Solubility of two vegetable oils in supercritical CO₂. *J. Supercrit. Fluids* (in press).
16. 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).
17. Uchytíl P., Schramm O., Seidel-Morgenstern A.: Influence of the transport direction on gas permeation in two-layer ceramic membranes. *J. Membr. Sci.* (in press).
18. Vachtová J., Heyberger A., Mrnka M., Procházka J.: Extraction of sulfuric acid with trialkylamine in a mixed diluent. *Ind. Eng. Chem. Res.* 38, 2028-2035 (1999).

Review papers

19. Uchytíl P.: Použití anorganických a polymerních membrán pro pervaporaci. (Czech) Application of inorganic and polymeric membranes for pervaporation. *Chem. Listy* (in press).

Monographs

20. Svoboda K., Roček J., Čermák Ji.: Možnosti odlučování submikronových částic prachu z odpadních plynů a spalin. (Czech) Possibilities of removal of submicron dust particles from flue and waste gases. Skripta pro postgraduální studium VŠCHT Praha, 63 pp. (1999).
21. Katz S., Staněk V., Landefeld C.: Cupola handbook. The basic cupola model. Chapter 28. Americal Foundrymen's Society, Des Plaines, Illinois, USA (in press).

Conferences

22. Jiříčný V., Ewans J. W.: Zinc-air fuel cells and zinc recovery-refueling system. 4th International Conference Zero Emission Vehicles, Karlovy Vary, Czech Republic, 17-18 June (1999).
23. Jiříčný V., Ewans J. W.: Regeneration of zinc particles from alkaline electrolytes in a spouted bed electrode. 22nd Meeting on Electrochemical Power Sources, Brno, Czech Republic, 30 August-2 September (1999).
24. Ondráček J., Jiříčný V., Svoboda P., Staněk V., Jakeš B.: Experimental techniques for RTD measurement in packed column. 12th Conference Process Control '99, Proceedings, pp. 193-196, High Tatras, Slovak Republic, 31 May-3 June (1999).
25. Staněk V., Ondráček J., Jiříčný V., Jakeš B.: Mathematical modelling of the structure of gas flow in a counter-current gas-liquid column. 12th Conference Process Control '99, Proceedings, pp. 107-110, High Tatras, Slovak Republic, 31 May-3 June (1999).
26. Staněk V.: Mathematical modeling of complex gas/liquid/solid systems. 1st International Conference on Process Development in Iron- and Steelmaking, Proceedings, Vol. 2., p. 33, Lulea, Sweden, 7-8 June (1999).

27. Svoboda P., Jiříčný V., Staněk V., Jakeš B.: Evaluation of transient hydrodynamic phenomena under a two-phase flow in packed bed. 12th Conference Process Control '99, Proceedings, pp. 111-114, High Tatras, Slovak Republic, 31 May-3 June (1999).
28. Vachtová J., Volaufová E., Heyberger A., Procházka J.: Amine extraction of sulfuric acid - effect of solvent composition. 26th International Conference SSChE, Proceedings, p. 109 Jasná, Slovakia, 24-28 May (1999).
29. Jeřábek K., Hanková L., Prokop Z.: Swollen-state morphology of hypersulfonated ion exchanger catalysts. "IEX 2000-Ion Exchange at the Millenium", Separation Science and Technology Group of the Society of Chemical Industry, Cambridge, Great Britain, (in press).

E. Hála Laboratory of Thermodynamics

Head: I. Wichterle
Deputy: K. Aim
Research staff: J. Kolafa, J. Linek, M. Lísal, I. Nezbeda, J. Pavlíček, M. Předota, M. Strnad, Z. Wagner
Visiting: M. Teodorescu
Part time: T. Boublík
Technical staff: S. Bernatová, Š. Psutka
PhD students: A. Babič, É. Kovács, 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
- Measurement of data for supercritical fluid extraction
- Determination of pressure–volume–temperature behaviour of liquids
- Thermodynamic modelling and processing of thermodynamic data
- Molecular simulations on model fluids and fluid mixtures
- Application of statistical–mechanical models to real fluids
- 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)

Molecular-simulated data for the two-centre Lennard–Jones dipolar model fluid along the vapour–liquid coexistence region have been used to assess the performance of an analytical (augmented van der Waals type) equation of state and the need for improvement in the parametric range of high elongations and dipole moments has been shown. The newly developed „reaction Gibbs ensemble Monte Carlo" simulation method has been successfully applied to predict the equilibrium properties of methanolic binary systems by using relatively simple molecular interaction model. The study on developing and testing analytical equations

of state for systems containing associating fluids based on primitive model of association has continued. [Refs. 6-9, 11, 12, 21, 25, 26, 34, 38]

Equilibrium behaviour of fluids constituted of anisotropic molecules

(K. Aim, joint project with CU; supported by GA CR, grant No. 203/97/0241)

By using the model of rod-like (possibly dipolar) molecules interacting by way of Kihara potential, the second-order perturbation theory for fluids constituted of anisotropic molecules has been successfully applied to calculate (i) the excess properties of mixing in binary systems of linear alkanes (differing in chain length), (ii) state and phase behaviour for a series of linear 1-chloroalkanes, and (iii) the excess properties of mixing in binary systems of the type linear alkane plus linear chlorinated hydrocarbon. Apparatus for the measurement of densities of liquid mixtures in the range from normal to high pressures has been calibrated and used (i) to complete the measurements of excess volume data at normal pressure for a series of binary systems of the type linear alkane (C₅ to C₈) plus linear chlorinated hydrocarbon (C₃ to C₆) and (ii) to determine the densities of n-heptane + 1-chloropentane mixtures at temperatures up to 330 K and pressures up to 400 bar. [Refs. 4, 23, 29, 35-37, 40]

Phase and state behaviour of fluid systems

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

Experimental: Systematic studies on relevant pure-compound vapour pressures (by high precision comparative ebulliometry) and on vapour-liquid equilibria (by dynamic still) have been conducted for a series of binary and ternary systems of the type ether + alkanol + hydrocarbon. Data processing: The performance of group contribution predictive methods (UNIFAC and DISQUAC) has been evaluated for the selected binary and ternary systems (including also the ketone + chloroalkane type systems) and new subsets of interaction parameters have been established. Data bases: Vapour-liquid equilibrium data bibliography has been supplemented by data covering year 1999 (and prepared for publishing as a book and in electronic form in 2000). [Refs. 1, 20, 31-33, 41, 45-48]

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

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

We have focused on methodology and formulated a perturbation expansion, tested its convergence and feasibility of its individual steps. Very extensive computer simulations have been carried out to examine in detail the effect of the range of intermolecular interactions on the orientation arrangement of water molecules in the bulk phase. [Ref. 14, 28]

Behaviour of liquids at very high pressures: Theory and applications

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

The first step towards the goal of the project is an accurate description of a suitably chosen reference system. We have developed and tested a new equation of state for a binary mixture of additive hard spheres which performs better even for a large diameter ratio than existing equations. [Refs. 2, 11]

Water cleanup using oxidation

(I. Nezbeda, joint project with L. L. Lee, University of Oklahoma, Norman; supported by National Science Foundation, program COBASE)

The concept of primitive models has been extended to dilute aqueous mixtures. Solutions of apolar fluids have been studied and it has been shown that the model predicts, unlike

existing engineering equations of state, all specific features of solubility in water including a maximum in the Henry's law constant. [Ref. 27]

Molecular thermodynamics of polar and associating fluid mixtures

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

Investigations pursued two paths. (1) A system of dipolar two-center Lennard–Jones fluids has been studied by a physically-based equation of state and computer simulations. (2) An equation of state, based on previous suggestions of Nezbeda and Pavlíček (Fluid Phase Equil. 116 (1996), 530) has been examined with respect of its ability to fit the critical properties. Encouraging results have been obtained and this part of the project will be one focus of the near future research. [Refs. 25]

Phase equilibria in systems with chemical reaction

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

Vapour–liquid equilibria are being studied in systems where chemical reaction takes place. The esterification reaction acetic acid + isopropyl alcohol \rightleftharpoons isopropyl acetate + water has been selected as a model system and experimental data were determined at 80 °C. A new simulation method (Reaction Ensemble Monte Carlo) has been proposed and used for thermodynamic modelling of isobutene + butane + methanol + MTBE reactive distillation. [Ref. 10, 12, 42, 45]

International co-operations

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

University of Guelph, Guelph, Canada: Molecular based modeling of systems with phase and chemical equilibria

University of Erlangen, Erlangen, Germany: Equation of state and chemical equilibrium

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

Visits abroad

I. Nezbeda: University of Oklahoma, Norman, USA (2 months); University of Leipzig, Leipzig, Germany; Agriculture University, Vienna, Austria; Technical University of Denmark, Lyngby, Denmark

J. Kolafa: Northwestern University, Evanston IL, USA (2 months)

J. Pavlíček: University of Erlangen, Erlangen, Germany (9 months)

M. Předota: University of Tennessee, Knoxville TN, USA (8 months)

Visitors

J. Fischer: Agriculture University, Vienna, Austria
H. V. Kehiaian: ITODYS, University of Paris VII, Paris, France
H. Knapp: Technical University, Berlin, Germany
A. Reiser: Brooklyn Polytechnic Institute, Brooklyn NY, USA
W. R. Smith, D. Drummond: University of Guelph, Guelph, Canada
J. Swaan Arons: University of Technology, Delft, The Netherlands
M. Teodorescu: Romanian Academy, Bucharest, Romania (8 months)

Teaching

T. Boublík: CU, courses "Basic physical chemistry", "Advanced chemical thermodynamics", and "Statistical thermodynamics"
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", "Introduction to molecular physics" (in English)

Publications

Papers

1. Dahmani O., Wichterle I.: Hard sphere expansion conformal solution theory with the Lennard-Jones (12-6) intermolecular potential. *Fluid Phase Equilib.* 161, 21-32 (1999).
2. Kolafa J.: Azeotropic phenomena in the global phase diagram of the Redlich-Kwong equation of state. *Phys. Chem. Chem. Phys.* 1, 5665-5670 (1999).
3. Kolafa J., Nezbeda I., Pavlíček J., Smith W. R.: Global phase diagrams of model and real binary fluid mixtures. II. Non-Lorentz-Berthelot mixture of attractive hard spheres. *Phys. Chem. Chem. Phys.* 1, 4233-4240 (1999).
4. Kovács É., Linek J.: Densities and excess volumes in binary mixtures of heptane with 1-chloropropane, 1-chlorobutane, 1-chloropentane, or 1-chlorohexane at 298.15 K. *Collect. Czech. Chem. Commun.* 64(3), 495-501 (1999).
5. Kovanda F., Kovács É., Koloušek D.: Removal of anions from solution by calcined hydrotalcite and regeneration of used sorbent in repeated calcination-rehydration-anion exchange processes. *Collect. Czech. Chem. Commun.* 64(9), 1517-1528 (1999).
6. Lísal M., Aim K.: Vapor-liquid equilibrium, fluid state, and zero-pressure solid properties of chlorine from anisotropic interaction potential by molecular dynamics. *Fluid Phase Equilib.* 161, 241-256 (1999).

7. Lísal M., Aim K., Vacek V., Černý F.: Vapour liquid equilibria of HFC and HCFC refrigerants from simple model fluid. *Acta Polytech.* 39, 17-37 (1999).
8. Lísal M., Budinský R., Vacek V., Aim K.: Vapour-liquid equilibria of alternative refrigerants by molecular dynamics simulations. *Int. J. Thermophys.* 20(1), 163-174 (1999).
9. Lísal M., Nezbeda I.: Pure fluid of homonuclear and heteronuclear square-well diatomics. I. Computer simulation study. *Mol. Phys.* 96(3), 335-347 (1999).
10. Lísal M., Nezbeda I., Smith W. R.: The reaction ensemble method for the computer simulation of chemical and phase equilibria. II. The Br₂+Cl₂+BrCl system. *J. Chem. Phys.* 110(17), 8597-8604 (1999).
11. Lísal M., Nezbeda I., Vörtler H. L.: Fluid-solid boundary of the compressed EXP-6 fluids. *Fluid Phase Equilib.* 154 (1), 49-54 (1999).
12. Lísal M., Smith W. R., Nezbeda I.: The accurate computer simulation of phase equilibrium for complex fluid mixtures. Application to binaries involving isobutene, methanol, MTBE, and n-butane. *J. Phys. Chem. B* 103, 10496-10505 (1999).
13. Mao Yi., Woenckhaus J., Kolafa J., Ratner M. A., Jarrold M. F.: Thermal unfolding of unsolvated cytochrome c: Experiment and molecular dynamics simulations. *J. Amer. Chem. Soc.* 121, 2712-2721 (1999).
14. Nezbeda I., Kolafa J.: Effect of short-and long-range forces on the structure of water: Temperature and density dependence. *Mol. Phys.* 97, 1105-1116 (1999).
15. Nezbeda I., Pavlíček J., Kolafa J., Galindo A., Jackson G.: Global phase behavior of model mixtures of water and n-alkanols. *Fluid Phase Equilib.* 158-160, 193-199 (1999).
16. Předota M., Nezbeda I.: Hydrophobic hydration at the level of primitive models. *Mol. Phys.* 96(8), 1237-1248 (1999).
17. Roháč V., Musgrove J. E., Růžička K., Růžička V., Zábanský M., Aim K.: Thermodynamic properties of dimethyl phthalate along the(vapour + liquid) saturation curve. *J. Chem. Thermodyn.* 31(8), 971-986 (1999).
18. Roháč V., Růžička V., Růžička K., Poledníček M., Aim K., Jose J., Zábanský M.: Recommended vapour and sublimation pressures and related thermal data for chlorobenzenes. *Fluid Phase Equilib.* 157(1), 121-142 (1999).
19. Slovák J., Koga K., Tanaka H., Zeng X. C.: Confined water in hydrophobic nanopores: Dynamics of freezing into bilayer ice. *Phys. Rev. E* 60, 5833-5840 (1999).
20. Aim K.: Vapor pressures of 2-chlorotoluene and 4-chlorotoluene and relative volatility in their binary system. *Thermochim. Acta* (in press).
21. Aim K.: On practical equations of state for methanol based on molecular theory. *Fluid Phase Equilib.* (in press).
22. Kettler M., Strnad M., Nezbeda I., Vörtler H. L.: Higher n-alkanes modeled as Kihara fluids: coexistence properties from simulation and theory. *Fluid Phase Equilib.* (in press).
23. Kovács É., Linek J.: Excess molar volumes of (alkane+1-chloroalkane) at T = 298.15 K. *J. Chem. Thermodyn.* (in press).
24. Linek J., Kovács É.: Excess molar volumes in systems alkane-1-chloroalkane. *Chem. Pap* (in press).
25. 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.* (in press).
26. Nezbeda I., Aim K.: A general method improving phase equilibrium calculations from pressure-explicit equations of state. *Fluid Phase Equilib.* (in press).
27. Nezbeda I.: Solubility of apolar fluids in water: A molecular model and theory. *Fluid Phase Equilib.* (in press).

28. Nezbeda I.: On the role of short- and long-range forces in aqueous systems. *J. Mol. Liq.* (in press).
29. Pavlíček J., Boublík T., Aim K.: Fluids of the Kihara molecules II. Binary mixtures of n-alkanes. *J. Phys. Chem.* (in press).
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31. 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.* (in press)
32. 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.* (in press).

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Conferences

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36. Aim K.: Properties of real fluid from simple interaction potentials. E. Hála Symposium on Thermodynamics, Prague, 7-9 October (1999).
37. Aim K., Kovács É., Linek J.: New experimental data of excess molar volumes for 16 binary systems of the type linear alkane + 1-chloroalkane. 1st IUPAC Workshop on Thermochemical, Thermodynamic and Transport Properties of Halogenated Hydrocarbons and Mixtures, Proceedings, pp. 75-76, Pisa, Italy, 15-18 December (1999).
38. Aim K., Pavlíček J.: Mixture properties of binary systems of the type linear alkane + 1-chloroalkane from the perturbation theory applied to model fluid of dipolar convex molecules. 1st IUPAC Workshop on Thermochemical, Thermodynamic and Transport Properties of Halogenated Hydrocarbons and Mixtures, Proceedings, pp. 32-33, Pisa, Italy, 15-18 December (1999).
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40. Linek J., Kovács É.: Excess molar volumes in systems alkane + 1-chloroalkane. 26th International Conference SSChE, Proceedings, p. 55, Jasná, Slovakia (1999).
41. Linek J.: Bibliography of vapour-liquid equilibrium data. E. Hála Symposium on Thermodynamics, Prague, 7-9 October (1999).
42. Lísal M.: Computer simulation of systems with chemical reaction. E. Hála Symposium on Thermodynamics, Prague, 7-9 October (1999).
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- namics and Statistical Mechanics with Industrial Applications", p. 48, London, 14-16 April (1999).
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 47. Wagner Z.: Application of gnostic theory to physico-chemical data. E. Hála Symposium on Thermodynamics, Prague, 7-9 October (1999).
 48. Wichterle I.: Vapour-liquid equilibrium in two (alcohol + ether + hydrocarbon) systems consisting of uniform solution of structural groups. 16th Thermodynamics Conference "Thermodynamics and Statistical Mechanics with Industrial Applications", p. 25, London, 14-16 April (1999).
 49. Wichterle I.: Continuation of the Eduard Hála legacy. E. Hála Symposium on Thermodynamics, Prague, 7-9 October (1999).

Department of Catalysis and Reaction Engineering

Head: M. Zdražil
Deputy: P. Schneider
Research staff: D. Gulková, V. Hejtmánek, K. Jiráková, R. Ponec, B. Sow, H. Šnajdaufová,
O. Šolcová, Z. Vít
Part time: L. Beránek, L. Fiala, A. Galík, A. Galíková, K. Klusáček
PhD students: J. Cinibulk, T. Klicpera, 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)

Complex analysis of pore structure of a broad set of industrial porous solids (monodisperse pore-size distribution, bi- and polydisperse pore-size distributions, with micropores, mesopores and macropores, etc.) is performed by standard textural analysis methods and non-standard transport measurement methods. The nitrogen physisorption, mercury porosimetry, helium pycnometry and liquid-expulsion permoporometry are used for standard textural analysis and multicomponent counter-current isobaric diffusion and gas permeation under non-steady state conditions are applied for non-standard transport measurement methods. The obtained data are mutually correlated. The simplest way for obtaining transport characteristics of porous solids, that are necessary for modern process and simulation control, is drawn from these correlations. [Ref. 16, 27, 30]

Graham cell for multicomponent gas diffusion in porous solids

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

Multicomponent diffusion of binary and ternary mixtures of inert gases (hydrogen, helium, nitrogen, argon) in an industrial catalysts (ICI) was studied in a diffusion cell in which the net diffusion flux of counter-currently diffusing components can be simply determined. Due to the influence of natural convection, attention had to be paid to mixing of gases in the cell compartments. A numerical algorithm was set up for evaluation of parameters of the Mean Transport-Pore Model; these parameters are material properties of the porous solid, i.e., are independent of the measurement conditions and kind of diffusing gases. [Refs. 5, 26, 39, 40]

Dynamics of the system: amines - aluminium oxide

(K. Klusáček)

Gravimetric transient response study of the adsorption, desorption and of deamination reaction revealed that the phenomenon known as the stop-effect is essentially influenced by the reaction products. The study of the kinetics of adsorption of propylamine and of desorption of the deamination products ammonia and propylene was therefore undertaken. The kinetic models of the adsorption and desorption of these components were worked out. [Ref. 3]

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 reaction of high surface area MgO with the slurry of $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}$ /methanol was used for the preparation of high surface area MoO_3/MgO catalysts. Various versions of this new technique were studied and the catalysts were tested in hydrodesulphurization of benzothiophene. The activity of the best MoO_3/MgO catalysts was comparable to the activity of conventional $\text{MoO}_3/\text{Al}_2\text{O}_3$ system. [Refs. 6, 18, 34, 41, 42]

The reaction of alumina surface OH groups with MoO_3 during slurry impregnation was studied using titration of OH groups with dimethylzinc. The stoichiometry of the reaction and surface coverage by molybdena species in $\text{MoO}_3/\text{Al}_2\text{O}_3$ catalysts was determined. [Ref. 13]

Iridium promoted molybdenum sulphide hydrodenitrogenation catalysts

(Z. Vít)

The preparation of alumina supported iridium sulphide catalysts was optimized. The catalysts exhibited high activity and selectivity in hydrodenitrogenation. Addition of iridium to conventional $\text{Mo}/\text{Al}_2\text{O}_3$ sulphide catalyst improved activity and selectivity to hydrodenitrogenation in parallel to hydrodesulphurization and hydrodenitrogenation. [Refs. 2, 15, 29]

Catalytic combustion of volatile organic compounds

(K. Jiráková, supported by GA ASCR, grant A4072904)

Catalytic combustion of model organic compound (toluene, ethanol) was studied with respect to the catalyst composition and the way of its preparation. Platinum catalysts prepared by microemulsion method, especially those containing low concentrations of platinum, showed the highest oxidation activity. $\text{Cu}/\text{Mg}/\text{Al}$ hydrotalcites and supported phosphomolybdic acids were prepared and their properties examined from the point of view of their use as potential oxidation catalysts. [Refs. 20, 32, 33, 36, 38]

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

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

12-Phosphomolybdic acid supported on hexagonal mesoporous silica showed enhanced hydrodesulphurization activity as compared with the catalysts prepared in the same way on alumina or amorphous silica. Zirconium incorporated into the mesoporous silica led to increased acidity and better molybdenum dispersion. Some alkali cations of phosphomolybdic acid stabilize polymeric structure of the active phase and increase its hydrodesulphurization activity. Introduction of lithium leads to the formation of lacunar heteropoly anion with defect Keggin structure. Activity of such catalyst in thiophene reaction is twice higher than that of the catalyst without lithium. [Refs. 19, 25, 35, 38]

Theoretical analysis and chemical applications of pair density matrices

(R. Ponec, supported by ICPF ASCR)

The project deals with the exploitation of pair densities as a new means of the analysis of the role of electron pairing in chemical bonds. Consistent with this general philosophy, several new methodologies for the analysis and visualization of bonding in molecules with complex bonding patterns were proposed. The examples are the electron deficient systems with multicenter bonds, hypervalent molecules or molecules with open shells. [Refs. 1, 7-12, 14, 21-24, 28, 37]

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

Catalytic oxidation of VOC and Catalysis over sulphides: Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

Visits abroad

R. Ponec: University of Pais Vasco, Bilbao, Spain (2 weeks)

R. Ponec: University of Hannover, Hannover, Germany (2 months)

Visitors

R. Bochicchio, University of Buenos Aires, Argentina

A. Spojakina, Institute of Catalysis, Sofia, Bulgaria

Teaching

- K. Jiráťová: PICT, postgraduate course "Preparation of heterogeneous catalysts"
R. Ponec: CU, courses "Reaction mechanisms in organic chemistry"
P. Schneider: PICT, postgraduate courses "Texture of porous solids"
M. Zdražil: PICT, postgraduate course "Preparation of heterogeneous catalysts"
K. Klusáček: PICT, postgraduate course "Nonstationary methods in heterogeneous catalysis"

Publications

Papers

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3. Galík A., Galíková A., Klusáček K.: Gravimetric transient response study of adsorption and reaction of propylamines on alumina. *Chem. Eng. Sci.* 54, 3495-3502 (1999).
4. Gulková D., Zdražil M.: Synergism between Ni and W in the Ni-W/C sulfide catalyst in hydrodenitrogenation of pyridine and hydrodesulfurization of thiophene. *Collect. Czech. Chem. Commun.* 64(4), 735-746 (1999).
5. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: adsorbable gases. *Chem. Eng. J.* 74(3), 171-179 (1999).
6. Klicpera T., Zdražil M.: High surface area MoO₃/MgO: preparation by the new slurry impregnation method and activity in sulphided state in hydrodesulphurization of benzothiophene. *Catal. Lett.* 58, 47-51 (1999).
7. Ponec R., Bochicchio R.: Nonlinear pair population analysis. The study of basis set dependence. *Int. J. Quant. Chem.* 72, 127-137 (1999).
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9. Ponec R., Duben A. J.: Electron pairing and chemical bonds. Bonding in hypervalent molecules from the analysis of the Fermi holes. *J. Comput. Chem.* 20(8), 760-771 (1999).
10. Ponec R., Amat L., Carbó-Dorca R.: Similarity approach to LFER. Substituent and solvent effect on the acidities of carboxylic acids. *J. Phys. Org. Chem.* 12, 447-454 (1999).
11. Ponec R., Amat L., Carbó-Dorca R.: Molecular basis of quantitative structure-properties relationships (QSPR): A quantum similarity approach. *J. Comput.-Aided Mol. Des.* 13, 259-270 (1999).
12. Torre A., Lain L., Bochicchio R., Ponec R.: On the nature of nonclassical bonds in closo-boranes: A nonlinear population analysis approach. *J. Comput. Chem.* 20, 1085-1090 (1999).
13. Vít Z.: Estimation of the molybdena coverage in MoO₃/alumina catalysts from residual OH groups. *Surf. Interface Anal.* 27, 861-864 (1999).
14. Bochicchio R., Lain L., Torre A., Ponec R.: Picture of bonding impropionated phosphorus and arsenic clusters. Detection and localization of 3-center bonds from the generalized population analysis. *Croat. Chem. Acta* (in press).

15. Cinibulk J., Vít Z.: Selective Mo-Ir/Al₂O₃ sulfide catalysts for hydrodenitrogenation. *Appl. Catal.* (in press).
16. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Determination of transport parameters of porous catalysts using unsteady permeation of gases. *Chem. Pap.* (in press).
17. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. *Catal. Lett.* (in press).
18. Klicpera T., Zdražil M.: Preparation of high surface area MoO₃/MgO by the reaction of MgO with slurry of ammonium heptamolybdate in methanol and its activity in hydrodesulphurization of benzothiophene. *J. Catal.* (in press).
19. Kostova N. G., Spojakina A. A., Dimitrov L. D., Petrov L. A., Šolcova O., Jiráťová K.: Zirconium-containing mesoporous silicates modified with 12-phosphomolybdic acid. *Microporous and Mesoporous Mater.* (in press).
20. Kovanda F., Jiráťová K., Rymeš J., Koloušek D.: Characterization of activated Cu/Mg/Al hydrotalcites and their catalytic activity in toluene combustion. *Appl. Clay Sci.* (in press).
21. Ponec R., Roithová J., Sannigrahi A. B., Lain L., Torre A., Bochicchio R.: On the nature of multicenter bonding in simple atomic clusters. *Theochem* (in press).
22. Ponec R., Roithová J.: Domain averaged Fermi holes - a new means of visualization of chemical bonds. *Bonding in hypervalent molecules. J. Comput. Chem.* (in press).
23. Ponec R., Roithová J., Haas Y.: Mechanism of gas phase ethene-ozone reaction and concomitant processes. Theoretical study. *Eur. J. Chem.* (in press). [23720]
24. Ponec R., Torre A., Lain L., Bochicchio R.: Multicenter bonding in open-shell systems. A nonlinear population analysis approach. *Int. J. Quantum Chem.* (in press).
25. Spojakina A. A., Kostova N. G., Jiráťová K.: Alkali cations effect on surface properties of silica-supported 12-phosphomolybdic acid and thiophene conversion on it. *Appl. Catal.* (in press).
26. Šolcová O., Šnajdaufová H., Hejtmánek V., Schneider P.: Textural properties of porous solids in relation to gas transport. *Chem. Pap.* (in press).
27. Šolcová O., Šnajdaufová H., Hejtmánek V., Schneider P.: Characterisation of porous solids for gas transport. *Stud. Surf. Sci. Catal.* (in press).

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28. Amat L., Carbó-Dorca R., Ponec R.: Simple linear QSAR models based on quantum similarity measures. 4th Girona Seminar on Molecular Similarity, Book of Abstracts, p. 36, Girona, Spain, 5-7 June (1999).
29. Cinibulk J., Vít Z.: Selective Mo-Ir/Al₂O₃ sulfide catalysts for hydrodenitrogenation. XXXIst Symposium on Catalysis, Book of Abstracts, p. Po10, Prague, 1-2 November (1999).
30. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Permeation of gas in industrial porous catalysts. 26th International Conference SSChE, Proceedings, p. 124, Jasná, Slovakia, 24-28 May (1999).
31. Hudec P., Smiešková A., Žídek Z., Schneider P.: Micropore t-plot analysis using the C(BET) parameter. 4th European Congress on Catalysis EUROPACAT-IV, Book of Abstracts, p. 388, Rimini, Italy, 5-10 September (1999).
32. Jiráťová K.: Microemulsion method for preparation of supported Pt nanoparticles and their use in combustion of VOC. 4th European Congress on Catalysis EUROPACAT-IV, Book of Abstracts, p. 834, Rimini, Italy, 5-10 September (1999).

33. Jiráťová K., Rymeš J., Sow B., Kovanda F., Koloušek D.: Oxidation activity and physical properties of activated Cu/Mg/Al hydrotalcites. XXXIst Symposium on Catalysis, p. Po12, Prague, 1-2 November (1999).
34. Klicpera T., Zdražil M.: Sulphide catalysts supported on magnesium oxide. XXXIst Symposium on Catalysis, p. Po11, Prague, 1-2 November (1999).
35. Kostova N. G., Spojakina A. A., Jiráťová K., Šolcová O., Dimitrov L. D., Petrov L. A.: Hexagonal mesoporous silicates with and without Zr as supports for HDS catalysts. 4th European Congress on Catalysis EUROPACAT-IV, Book of Abstracts, p. 631, Rimini, Italy, 5-10 September (1999).
36. Kovanda F., Jiráťová K., Rymeš J., Koloušek D.: Characterization of activated Cu/Mg/Al hydrotalcites. Conference of the European Clay Groups Association Euroclay 1999, Book of Abstracts, p. 104, Krakow, Poland, 5-9 September (1999).
37. Ponec R., Amat L., Carbó-Dorca R.: Molecular basis of structure-activity relationships. 4th Girona Seminar on Molecular Similarity, Book of Abstracts, p. 29, Girona, Spain, 5-7 July (1999).
38. Spojakina A. A., Kostova N. G., Sow B., Savova D. N., Stamenova M. W., Jiráťová K.: Thiophene hydrogenolysis and ethanol oxidation on the SiO₂ supported 12-PMoV-mixed heteropoly compounds. 4th European Congress on Catalysis EUROPACAT-IV, Book of Abstracts, p. 779, Rimini, Italy, 5-10 September (1999).
39. Šnajdaufová H., Šolcová O., Hejtmánek V., Schneider P.: Textural properties of porous solids in relation to gas transport. 26th International Conference SSChE, Proceedings, p. 125, Jasná, Slovakia, 24-28 May (1999).
40. Šolcová O., Šnajdaufová H., Hejtmánek V., Schneider P.: Characterisation of porous solids for gas transport. 5th International Symposium on the Characterisation of Porous Solids, Heidelberg, Germany, 30 May-2 June (1999).
41. Zdražil M.: Supported MoO₃ catalysts: preparation by the new "slurry impregnation" method and activity in hydrodesulphurization. 4th European Congress on Catalysis EUROPACAT-IV, Book of Abstracts, p. 0/02/02, Rimini, Italy, 5-10 September (1999).
42. Zdražil M.: Preparation of supported molybdenum catalysts by new slurry impregnation method. XXXIst Symposium on Catalysis, p. Po6, Prague, 1-2 November (1999).

Department of Multiphase Reactors

Head:	J. Drahoš
Deputy:	J. Zahradník
Research staff:	M. Fialová, J. Slezák, M. Růžička, V. Sobolík, J. Tihon, O. Wein Part time: V. Pěnkavová, J. Vrba
Technical staff:	S. Nováková, V. Tovchigrechko Part time: J. Kubešová, A. Zemek
PhD student:	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. Identification of hydrodynamic mechanisms causing the instability of the homogeneous bubbling regime, investigation of the character of this instability. [Refs. 3, 10, 12, 13, 22, 23, 25]

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. [Ref. 26]

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. 4, 5, 14, 15, 27]

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

(J. Tihon, supported by GA ASCR, grant No. A4072914/1999)

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. 28-30]

The effect of liquid phase properties on the rate of gas-liquid mass transfer in reactors with ejector gas distributors

(J. Zahradník, joint project with PICT, Prague; supported by the GA CR, grant No. 104/97/1170)

Hydraulic characteristics of the ejector loop reactor have been determined in a wide viscosity range of the liquid medium. The effect of viscosity on the rate of energy dissipation, the gas suction rate and the gas hold-up in ejector loop reactors have been examined. Residence time distribution of gas phase has been measured in electrolyte and viscous batches using the pulse response technique. Studies of bubble coalescence in viscous aqueous media proved that coalescence in such media could be significantly modified by addition of surfactants (aliphatic alcohols). [Refs. 7-9]

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

(J. Zahradník, joint project with UMIST Manchester, UK, Inst. Chem. Eng., Bulgarian Acad. Sci., 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. 7, 8, 19, 24]

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

(J. Zahradník, 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. 1, 3, 10-13, 20, 21, 25]

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
Inst.Chem. Eng., 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

Visits abroad

J. Drahoš: The State University of New Jersey, U.S.A.; University of Sao Paulo, Brazil;
University of Ljubljana, Slovenia; TU Delft, The Netherlands; Martin Luther University,
Halle, Germany; STU Bratislava, Slovakia
M. Fialová: Aristotle University Thessaloniki, Greece; Performance Fluid Dynamics Ltd.,
Dublin, Ireland
M. Růžička: TU Delft, The Netherlands
V. Sobolík: University of La Rochelle, France (11 months); University of Kobe, Japan
(1 month)
J. Tihon: University of Notre Dame, U.S.A.; CNRS UPR 15, Paris, France; CRTT Saint
Nazaire, France
J. Vejražka: LEGI / IMG, Grenoble, France (3 months)
O. Wein: University of Calgary, Canada (3 months)
J. Zahradník: Aston University, Birmingham, UK; University of Birmingham, Birmingham,
UK; UMIST Manchester, UK; TU Delft, The Netherlands; CSIR, Johannesburg, South
Africa; University of Minho, Braga, Portugal

Visitors

S.-P.Lin, University of Clarkson, U.S.A.
N.H. Thomas, Aston University, Birmingham, UK
M. Valeva, Inst. Chem. Eng., Bulgarian Acad. Sci., Sofia, Bulgaria
S. Endoh, NIRE, Tsukuba, Japan
K. Yoshida, Tokyo University, Japan

Teaching

J. Drahoš: PICT, course "Fluid Mechanics"

O. Wein: TU Brno, course "Principles of Rheology"

J. Zahradník: TU Brno, course "Bioengineering"; PICT, postgraduate course "Multiphase Reactors"

Publications

Papers

1. Freitas C., Fialová M., Zahradník J., Teixeira J. A.: Hydrodynamic model for three-phase internal- and external-loop airlift reactors. *Chem. Eng. Sci.* 54(21), 5253-5258 (1999).
2. Punčochář M., Drahoš J.: Fractal geometry: A tool for fuzzy reasoning. *Int. J. General Systems* 27, 397-406 (1999).
3. Růžička M., Drahoš J., Zahradník J., Thomas N. H.: Natural modes of multi-orifice bubbling from a common plenum. *Chem. Eng. Sci.* 54(21), 5223-5229 (1999).
4. Sobolík V.: Electrochemical study of Taylor-Couette flow by limiting diffusion current method. *Collect. Czech. Chem. Commun.* 64(7), 1193-1210 (1999).
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29. Tihon J.: Wavy film flow of Non-Newtonian liquids down an inclined plane. IUTAM Symposium, Abstract, p. 47, University of Notre Dame, USA, 7-9 July (1999).
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Department of Biotechnology and Environmental Processes

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

- Pilot-scale sorption and biodegradation of PCBs from ground water
- Hydrogenation of low molecular weight polybutadienes
- Microwave processing of glass

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.

Dehalogenation of polychlorinated biphenyls by Fenton's reagent

(J. Včelák, project supported by GA CR, grant No. 203/97/1173)

The study in the last year was focused on reactions of Fenton's reagent with PCA's and PCB's in catalysed biphasic systems. The selectivity of polychloroaromatic substrates producing polychlorophenols was estimated together with products of the phase transfer catalyst decay. The reactivity of PCB mixtures with Fenton's reagent was observed to be too small to complete their total dehalogenation. The distribution ratio of chlorophenols and polychlorophenols between water and organic solvents was determined to improve quantitative description of reaction systems. [Refs. 22, 41, 42]

Technology of organic chlorinated pollutants biodegradation

(G. Kuncová, joint project with PICT, supported by GA CR, grant No. 104/97/1212)

The optical detection of polychlorinated biphenyls based on production of long lasting yellow intermediates by aerobic microorganisms *Pseudomonas sp. 2*, immobilized on glass carrier and in alginate beads coated with silica layer was studied. Sensitivity of the method depends on relations between the number of immobilized cells and concentration of polychlorinated biphenyls. The method enabled detection of polychlorinated biphenyls selectively in water with mineral oil and chlorinated hydrocarbons. The application of liquid core waveguide spectrophotometer for measurement of concentration of yellow intermediates increased the sensitivity hundred times compared to that with standard spectrophotometer equipped with 1 cm cell. [Refs. 27, 34-36]

Microwave activation of chemical reactions on solid catalysts and supports

(M. Hájek, supported by GA CR, grant No. 203/97/1175)

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. In addition to the main project an activation method of photochemical reactions by microwave irradiation has been studied using electrodeless lamps and a new photoreactor for organic synthesis was developed [Refs. 1, 5, 19, 32, 33, 38, 39]. In applied research, a new technology for manufacture of glass by microwave energy has been developed [Refs. 3, 4, 23, 25, 31].

Catalysis by transition metal complexes with azine ligands

(J. Čermák, joint project with CU, supported by GA CR, grant No. 203/97/1157)

Methallylchloropalladium complexes of a series of novel azine diphosphine ligands with different alkyl and aryl substituents on phosphorus atoms were prepared and their 2D ¹H NOESY NMR spectra measured with the aim of semiquantitative determination of the steric parameters of the donor site. Equilibrium between nickel(0) complexes with chelating

bis(diphenylphosphino)pinacoloneazine was investigated and unexpected thermodynamic control of the reaction revealed. Electrochemical vs. thermal activation of an alkyne ligand in palladium(0) complex with chelating (*Z,Z*)-bis(diphenylphosphino)pinacoloneazine was studied and the mechanisms of formation of different products elucidated. The *cis*-vinyl complex formed by the thermal activation is an active catalyst for the Heck reaction. [Refs. 13, 16, 17, 29, 30]

Novel techniques for implementation of immobilized biocatalysts in industrial processes (G. Kuncová, supported under INCO-COPERNICUS project Erbic15CT98)

The main objective of this project, which started in October 1998, is facilitation of 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. 11, 12, 28]

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. [Refs. 28, 40]

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

(J. Hetflejš, joint project with Inst. Macromol. Chem. ASCR, supported by GA ASCR, grant No.4072902/99)

The subject of the project is to find a broad variety of targeted chemical modifications of liquid polybutadienes (hydrophilization of the chain through etherification, hydrogenation of residual double bonds, attachment of antioxidants and stabilizers) and thus to prepare novel materials interesting both for basic research and applications. The study of mesoscopic structures of block siloxane-butadiene copolymers is expected to yield important data concerning organized supermolecular structures without entanglements.

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

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

Novel perfluoroalkyl-substituted tetramethylcyclopentadienes (Cp^fH) were synthesized. Their rhodium(III) and rhodium(I) complexes of the types $[Cp^fRhCl_2]_2$ and $[Cp^fRhL_2]$ ($L_2 = 2 CO, 1,5-COD$), respectively, were prepared as fluorophilic analogs of known hydrogenation and hydrosilylation catalysts. The influence of perfluoroalkyl chain length on the solubility of the complexes and on the electronic properties of the ligands characterized by NMR and IR properties of ancillary ligands (CO and 1,5-COD) were studied. [Ref. 26]

International co-operations

Université de Paris-Sud, Paris, France: Activation of solvent-free reactions
Institute of Geotechnique, SAS, Košice, Slovakia: Microwave desulfurization of coal
National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania: Microwave assisted heterogeneous catalytic 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, USA (12 months)
S. Šabata: Instituto Superior Técnico, Lisbon, Portugal

Visitors

L. Perreux, Université de Paris-Sud, Paris, France
I. Murová, Institute of Geotechnique, SAS, Košice, Slovakia
M. Radoiu, National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania (10 months)
E. Esveld, Agrotechnical Research Institute ATO-DLO, Wageningen, The Netherlands
M.F.N.N. Carvalho, Instituto Superior Técnico, Lisbon, Portugal
S. Marseaut, Haute Ecole Lucia de Brouckere, Institute Meurice Chimie, Institut Supérieur Industriel, Brussels, Belgium (5 months)

Teaching

F. Kaštánek: TU Brno and PICT: courses "Bioengineering"

Publications

Papers

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3. Hájek M.: Mikrovlnné tavení skla. (Czech) Microwave processing of glass. *Sklář a Keramik* 49(9-10), 281-283 (1999).
4. Hájek M.: Mikrovlnná sklářská pec – spojení moderní technologie se sklářskou tradicí. (Czech) Microwave glass furnace - a connection of modern technology with glass tradition. *Sklář a Keramik* 49(9-10), 249-250 (1999).
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11. Brányik T., Kuncová G.: Changes in microbial respiration as a result of immobilization by sol-gel method and the use of silica gel in microbial sensor construction. *Biotechnol. Lett.* (in press).
12. 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.* (in press).
13. 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 $[\text{Pd}\{\text{PPh}_2\text{CH}-\text{C}(\text{Bu}^t)\text{NN}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2\}\{\text{C}(\text{CO}_2\text{Me})=\text{CH}(\text{CO}_2\text{Me})\}]$ and $[\text{Pd}\{\text{(Z, Z)PPh}_2\text{CH}_2\text{C}(\text{Bu}^t)=\text{NN}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2\}\{\text{C}(\text{CO}_2\text{Me})=\text{C}(\text{CO}_2\text{Me})\}]$. *J. Organometal. Chem.* (in press).
14. Církva V., Gaboyard M., Paleta O.: Fluorinated epoxides. 5. Highly selective synthesis of diepoxides from alfa, omega-diiodoperfluoroalkanes. Regioselectivity of nucleophilic epoxide-ringopening and new amphiphilic compounds and monomers. *J. Fluorine Chem.* (in press).
15. Církva V., Bohm 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.* (in press).
16. Čermák Jan, Šabata S., Blechta V., Shaw B. L.: Nickel(0) and palladium(0) complexes with (Z, Z)- $\text{Ph}_2\text{PCH}_2\text{C}(\text{t-Bu})=\text{NN}=\text{C}(\text{t-Bu})\text{CH}_2\text{PPh}_2$. Alkyne to alkenyl conversion in $[\text{Pd}(\text{H}_3\text{COCC}=\text{CCOOCH}_3)\{\text{(Z, Z)-Ph}_2\text{PCH}_2\text{C}(\text{t-Bu})=\text{NN}=\text{C}(\text{t-Bu})\text{CH}_2\text{PPh}_2\}]$. *Collect. Czech. Chem. Commun.* (in press).
17. Čermák Jan, Kvíčalová M., Šabata S., Blechta V., Vojtíšek P., Podlaha J.: Disphosphinoazines with phosphine groups of various sizes and their (2-methylpropenyl)palladium complexes. *Appl. Organomet. Chem.* (in press).
18. Čermák Jan, Kvíčalová M., Blechta V.: Pentamethylcyclopentadienyl rhodium(I) complexes incorporated into porous polysiloxanes prepared by a sol-gel process - catalysts for hydrogenation of crotonic acid in water. *Appl. Organomet. Chem.* (in press).
19. Hájek M., Radoiu M.: Microwave activation of catalytic transformation of t-butylphenols. *J. Mol. Catal.* (in press).

20. 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).
21. Podlaha J., Císařová I., Kvíčalová M., Schraml J.: Self-assembly of 4-nitrobenzhydroxamic acid in the crystal. *Supramol. Chem.* (in press).
22. Včelák J., Řeřicha R., Hetflejš J.: Metal complex-catalyzed dechlorination of chloroarenes by SDMA-side reactions. *Appl. Organometal. Chem.* (in press).

Review papers

23. 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

24. Kaštánek F.: Bioinženýrství. (Czech) Bioengineering. ACADEMIA, Prague (in press).

Czech patents

25. 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).

Conferences

26. Auerová K., Čermák Jan, Nguyen H. T. T., Blechta V.: The synthesis of metal complexes with cyclopentadienyl ligands containing perfluoroalkyl ponytails. XXXIst Symposium on Catalysis, p. Po18, Prague, 1-2 November (1999).
27. Brányik T., Kuncová G., Páca J.: Continuous degradation of phenol by cells encapsulated into silica gel. 9th European Congress on Biotechnology, Abstract ECB9/2815, Brussels, Belgium, 11-15 July (1999).
28. Brányik T., Kuncová G., Podrazký O., Szilva J., Klier D.: Optical probes in the process of PCB degradation. Advanced Study Course on Optical Chemical Sensors ASCOS 1999, Keynote 12, Neusiedl am See, Austria, 27-29 September (1999).
29. Carvalho M. F. N. N., Čermák Jan, Galvao A. M., Pombeiro A. J. L., Šabata S.: Synthesis, characterization and study of the electronic properties of $[\text{NiX}(\text{R}_2\text{PCH}_2\text{C}(\text{But})=\text{N}-\text{N}=\text{C}(\text{But})\text{CH}_2\text{PR}_2)]\text{Y}$. XIIIth FEICHEM Conference on Organometallic Chemistry, Book of Abstracts, p. P41, Lisbon, 29 August-3 September (1999).
30. Čermák Jan, Kvíčalová M., Petričkovič R., Šabata S., Blechta V., Vojtíšek P.: Disphosphinoazines with phosphine groups of various sizes and their (2-methylallyl)palladium complexes. XIIIth FEICHEM Conference on Organometallic Chemistry, Book of Abstracts, p. P46, Lisbon, 29 August-3 September (1999).
31. Hájek M.: Microwave processing of glass. 5th ESG Conference Glass Science and Technology for the 21st Century, Book of Abstracts, p. 180, Praha, 21-24 June (1999).
32. Hájek M.: Microwaves and catalysis. 7th International Conference on Microwave and High Frequency Heating, pp. 247-250, Valencia, Spain, 13-17 September (1999).
33. Hájek M., Radoiu M.: Microwave induced catalytic transformation of t-butylphenols. XXXIst Symposium on Catalysis, p. OP3, Prague, 1-2 November (1999).

34. Kuncová G., Poncelet D., Burkhard J., Demnerová K., Pazlarová J.: Biodegradation of polychlorinated biphenyls by immobilized microorganisms. 8th International Workshop on Bioencapsulation, Abstract, P-9, Trondheim, Norway, 14-17 September (1999).
35. Kuncová G., Berková D., Burkhard J., Demnerová K., Pazlarová J., Tříška J., Vrchotová N.: Optical detection of polychlorinated biphenyls. International Conference on Environmental Monitoring and Remediation Technologies II, Session 1, Boston, Massachusetts USA, 19-22 September (1999).
36. Langová M., Kochánková L., Burkhard J., Tříška J., Kuncová G.: Isolation and identification of metabolites of selected polychlorinated biphenyls. 1st Meeting on Chemistry and Life, Book of Abstracts, p. 188-189, Brno, Czech Republic, 9-10 September (1999).
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38. Radoiu M., Hájek M.: Microwave activation of montmorillonite KSF catalyst on the transformation of 2-t-butylphenols. XIth International Conference on Chemistry and Chemical Engineering, Book of Abstracts, p. PO 24, Bucharest, Romania, 30 October-2 November (1999).
39. Radoiu M. T., Hájek M.: Microwave induced catalytic transformation of t-butylphenols. 7th International Conference on Microwave and High Frequency Heating, pp. 251-254, Valencia, Spain, 13-17 September (1999).
40. Vaňková R., Kuncová G.: Two-dimensional fluorescence spectroscopy as a tool for estimation of growth and viability of immobilized plant cells. 8th International Workshop on Bioencapsulation, Abstract, P-10, Trondheim, Norway, 14-17 September (1999).
41. Včelák J., Czakóová M., Hetflejš J.: Chloroarene and PCB's oxidations by Fentons's reagent. XIIIth FEICHEM Conference of Organometallic Chemistry 1999, Book of Abstracts, p. P59, Lisboa, Portugal, 29 August-3 September (1999).
42. Včelák J., Řeřicha R., Hetflejš J.: Metal complex-catalyzed dechlorination of chloroarenes by SDMA-side reactions. XIIIth FEICHEM Conference of Organometallic Chemistry 1999, Book of Abstracts, p. P280, Lisboa, Portugal, 29 August-3 September (1999).

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Head: J. Smolík
Deputy: R. Fajgar

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. Cinibulková, J. Kugler, V. V. Levdanskij, P. Moravec,
J. Schwarz, V. Ždímal

PhD students: 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 fluidized bed combustion

(J. Smolík, supported by GA ASCR, grant No. A 2046904)

The project is aimed at study of composition and behaviour of minerals and inorganic elements during fluidized bed combustion in connection with their distribution and mode of occurrence. Special attention is 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.

The thermodynamic approach is also used to estimate partitioning of trace elements between various emission streams. [Refs. 3, 6-8, 10, 23]

Experimental study of the homogeneous nucleation kinetics in supersaturated vapors

(V. Ždímal, supported by GA CR, grant No. 104/97/1198)

A new method for studying kinetics of homogeneous nucleation in supersaturated vapors using a static diffusion chamber was developed and tested. The experiments in n-pentanol formed a part of an international comparative study, and proved high precision of the approach [Ref. 2, 26]. It enabled us to test validity of Kelvin equation for clusters consisting of several tens of molecules. A new model of growth and motion of a droplet in an anisotropic gaseous mixture has been derived [Ref. 11]. Another model, describing transport processes in associating vapors, has been used in vapors of acetic acid, cesium and sulphur. The original nucleation data in these systems have been obtained as well.

Gas phase synthesis of multicomponent nanoparticles

(P. Moravec, supported by GA ASCR, grant No. A 4072807)

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 mixed silica-alumina particles were prepared by decomposition of aluminium tri-*sec*-butoxide, titanium tetra-*iso*-propoxide and tetraethylortho-silicate. Particles were characterised by SEM, TEM and EDAX analysis. [Refs. 1, 4, 5, 18-20]

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

Visits abroad

J. Smolík: University of Helsinki, Finland

J. Smolík: University College, London, England

V.V. Levanskij: KRICT, Taejon, Korea

Visitors

M. Kulmala, University of Helsinki, Finland

S. Friedlander, UCLA, California, USA

P. Hopke, Clarkson College, USA

J.C. Barret, Royal Naval College, London, UK
I. Ford, University College, London, UK
P.E. Wagner, Institute of Physics, University of Vienna, Austria
S. Bakanov, Institute of Physical Chemistry, Moscow, Russia
A. Lushnikov, Karpov Institute, Moscow, Russia
D. Ahn, Kang-Ho, Hanyang University, Korea
M. Choi, Seoul National University, Korea
D. Kim, Yong Pyo, KIST, Korea
H.D. Jang, KIGAM, Korea

Publications

Papers

1. Levdansky V. V., Moravec P., Smolík J.: Deposition of substance from a gas mixture on aerosol particles. *J. Eng. Phys. Thermophys.* 71(4), 694-699 (Translated from *Inzhenerno-Fizicheskii Zhurnal*, 71(4), 698-703 (1998)) (1999).
2. Rudek M. M., Katz J. L., Videnský I. V., Ždímal V., Smolík J.: Homogeneous nucleation rates of n-pentanol measured in an upward diffusion cloud chamber. *J. Chem. Phys.* 111(8), 3623-3629 (1999).
3. Smolík J., Schwarz J., Veselý V., Sýkorová I., Kučera J., Havránek V.: Characterization of solid emissions from atmospheric fluidized-bed combustion of two Czech lignites. *Environ. Sci. Technol.* 33(20), 3543-3551 (1999).
4. Smolík J., Moravec P.: Aerosolové procesy pro přípravu práškových materiálů. (Czech) *Aerosol processes for synthesis of fine powders. Sklář a keramik* 49(3), 51-54 (1999).
5. 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).
6. Havránek V., Kučera J., Horáková J., Voseček V., Smolík J., Schwarz J., Sýkorová I.: Matrix effects in PIXE analysis of aerosols and ashes. *Biol. Trace Element Res.* (in press).
7. Kučera J., Havránek V., Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Šantroch J.: INAA and PIXE of atmospheric and combustion aerosols. *Biol. Trace Element Res.* (in press).
8. 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.* (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).
10. Sýkorová I., Bouška V., Smolík J., Schwarz J., Kučera J., Havránek V.: Influence of additives on emissions from the fluidized bed combustion of lignite. *Prospects for Coal Science in the 21st Century*, Shanxi Science & Technology Press, pp. 499-501 (1999).

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11. Bakanov S. P., Smolík J., Zaripov Sh. Kh., Ždímal V.: Mathematical model of motion of growing droplet in a thermal diffusion cloud chamber. *J. Aerosol Sci* 30, S1, S73-S74 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).

12. Džumbová L., Schwarz J., Smolík J.: Evaporation of water droplet in the humid atmosphere. *J. Aerosol Sci.* 30, S1, S337-S338 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
13. Hillamo R., Sillanpää M., Kerminen V. M., Schwarz J., Džumbová L., Kugler J., Smolík J., Brožová I., Bartáčková Z., Šantroch J., Hovorka J., Kučera J., Havránek V.: Composition and size of atmospheric aerosol in Prague. *J. Aerosol Sci.* 30, S1, S665-S666 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
14. Hillamo R., Mäkelä T., Schwarz J., Smolík J.: Collection characteristics of the model 25/0, 018/2 Berner low pressure impactor. *J. Aerosol Sci.* 30, S1, S901-S902 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
15. Hillamo R., Sillanpää M., Kerminen V.-M., Schwarz J., Džumbová L., Kugler J., Smolík J., Brožová I., Bartáčková Z.: Particle size distributions of gravimetric mass and composition of polluted urban aerosol. 18th Annual Conference AAAR'99, p. 153, Tacoma, Washington, USA, 11-15 October (1999).
16. Hovorka J., Veron A. J., Schwarz J., Džumbová L., Kugler J., Smolík J.: Stable lead isotope ratios in size-fractionated urban aerosols. *J. Aerosol Sci.* 30, S1, S383-S384 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
17. Kim H. Y., Kim H. C., Levdansky V. V., Moravec P., Smolík J.: Selective influence of electromagnetic fields on aerosol systems. *J. Aerosol Sci.* 30, S1, S321-S322 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
18. Levdansky V. V., Moravec P., Smolík J., Ždímal V.: Laser-assisted deposition of gas molecules on aerosol particles. E-MRS 1999 Spring Meeting, Book of Abstracts, p. A-33, Strasbourg, France, 1-4 June (1999).
19. Levdansky V. V., Moravec P., Smolík J., Ždímal V.: Growth of small particles in deposition from gas phase. 18th European Conference on Surface Science, Abstracts, Vol. 23G, Tu-P-052, Vienna, Austria, 21-24 September (1999).
20. Moravec P., Smolík J., Levdansky V. V.: Preparation of mixed $\text{Al}_2\text{O}_3\text{-SiO}_2$ fine particles by CVD method. *J. Aerosol Sci.* 30, S1, S353-S354 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
21. Schwarz J., Smolík J., Vakevā M., Kulmala M., Vesala T.: The influence of tetradecane vapors on water drop evaporation. *J. Aerosol Sci.* 30, S1, S399-S400 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
22. Schwarz J., Smolík J., Hillamo R., Mäkelä T.: Calibration of Berner low pressure impactors. 18th Annual Conference AAAR'99, p. 11, Tacoma, Washington, USA, 11-15 October (1999).
23. Smolík J., Schwarz J., Leitner J.: Matrix and trace elements behaviour in fluidised bed combustion - an equilibrium analysis. *J. Aerosol Sci.* 30, S1, S781-S782 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
24. Smolík J., Schwarz J., Veselý V., Punčochář M., Kugler J., Sýkorová I., Havránek V.: Composition of particulate emissions from fluidised bed combustion of charcoal. *J. Aerosol Sci.* 30, S1, S783-S784 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
25. Stratmann F., Ždímal V., Wilck M., Smolík J.: New 2-D coupled fluid flow, heat and mass transfer model for the description of thermal diffusion cloud chambers. *J. Aerosol Sci.* 30, S1, S75-S76 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
26. Ždímal V., Smolík J., Rudek M. M., Katz J. L.: Joint experiments on homogeneous nucleation: static diffusion chamber results. *J. Aerosol Sci.* 30, S1, S27-S28 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).

27. Smolík J., Schwarz J., Sýkorová I., Veselý V., Kugler J., Kučera J., Havránek V.: Vliv parametrů procesu na emise stopových prvků z fluidního spalování hnědého uhlí. (Czech) The influence of process parameters on trace elements emissions from fluidised bed combustion of lignites Ověřeno '99, pp. 133-138, Brno, 7.-10. 2.(1999).

Group of Hydrodynamics and Chemistry of Incineration

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

PhD students: M. Jochová

Technical staff: J. Ullrich

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 influence of additives on the release of heavy metals on fly ash from lignite combustion was investigated. Simultaneously, the effect of sulfur compounds (diluted and concentrated sulfur acid, sulfur dioxide with hydrogen peroxide) was explored for reduction of polyhalogenated dibenzo-p-dioxins and benzofurans emissions. The most efficient additive for PCDD/F dropping, we found, was the combination $\text{SO}_2 + \text{H}_2\text{O}_2$. Further, the influence of water on PCDD/F de novo synthesis and polyaromatic hydrocarbons formation was investigated. Experiments revealed strong influence of water injection into the flue gas on dioxins formation, whereas the concentration of PAHs was dropped. [Refs. 1, 5, 6, 10-12]

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

(V. Pekárek, supported by GA ASCR, grant No. A 4072901/1999)

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 safe landfilling seems to be only the time-limiting solution. The study of their detoxification by means of dehalogenation or destruction on catalytically active surfaces of inorganic sorbents is therefore a highly desirable ecological problem for the solution. The chemical reactions will be studied in the dependence on chemical composition of solid phase, amount and character of catalyzed phase, and on temperature by classical or microwave heating. The optimum solution of this problem will come out from the probable reaction mechanism. Owing to the fact that these compounds are firmly bound to the surfaces, the desorption studies are included, too. The experiments will be performed so that no "novosynthetic reactions" might occur. The project results would bring ideas for technological detoxification of toxic flue ashes from municipal waste incinerators. The model chemicals will be used also for the studies. [Refs. 3, 5, 10]

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.

International co-operation

NIRE, Tsukuba, Japan: Resources recycling in eastern Europe

Umeå University, Dept. of Environmental Chemistry, Umeå, Sweden: Emissions of persistent organic pollutants from spark engine

Visits abroad

M. Punčochář: Ohio State University, Columbus, USA; Carnegie Mellon University, Pittsburgh, USA

Visitors

S. Endoh: NIRE, Tsukuba, Japan

S. Marklund: Umeå University, Sweden

Publications

Papers

1. Grabic R., Marklund S., Pekárek V., Punčochář M., Ullrich J.: Effects of oxygen, sulphur dioxide, sulphuric acid and peroxides on formation of polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) on the MWI fly ash. *Organohalogen Compd.* 41, 251-254 (1999).
2. Punčochář M., Drahoš J.: Fractal geometry: A tool for fuzzy reasoning. *Int. J. General Systems* 27, 397-406 (1999).
3. Stach J., Pekárek V., Endršt R., Hetflejš J.: Dechlorination of hexachlorobenzene on MWI fly ash. *Chemosphere* 39(14), 2391-2399 (1999).
4. Yano T., Kikuchi R., Tsutsumi A., Yoshida K., Punčochář M., Drahoš J.: Nonlinear hydrodynamics of three-phase reactors. *Kagaku Kogaku Ronbunshu* 25, 530-534 (1999).
5. Pekárek V., Grabic R., Marklund S., Punčochář M., Ullrich J.: Effects of oxygen on formation of polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) on the extracted municipal waste incinerator fly ash in the presence of carbon and cupric salt. *Chemosphere* (in press).
6. Punčochář M., Drahoš J.: Limits of applicability of capillary model for pressure drop correlations. *Chem. Eng. Sci.* (in press).
7. Vrba J., Punčochář M., Drahoš J.: Fuzzy decomposition applied on logistic equation. *SAMS* (in press).
8. 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 PAHs, PCDDs, PCDFs, and PCBs emissions from spark engine fuelled with leaded gasoline. *Chemosphere* (in press).

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9. Drahoš J., Punčochář M.: Transition between the capillary and particulate models for pressure drop correlations. 27th Congress on Particulate Systems, Book of Abstracts, Campos do Jordao, Brazil, 18-21 October (1999).
10. Grabic R., Marklund S., Pekárek V., Punčochář M., Ullrich J.: Effects of oxygen, sulphur dioxide, sulphuric acid and peroxides on formation of polychlorinated biphenyls, dibenzo-p-dioxins and dibenzofurans on the MWI fly ash. 19th International Symposium on Halogenated Environmental Organic Pollutants and POPs, Venice, Italy, 12-17 September (1999).
11. Punčochář M., Veselý V.: The reduction of POP emissions by using of sulphur additives. 26th International Conference SSChE, Proceedings, p. 134, Jasná, Slovakia, 24-28 May (1999).
12. Smolík J., Schwarz J., Veselý V., Punčochář M., Kugler J., Sýkorová I., Havránek V.: Composition of particulate emissions from fluidised bed combustion of charcoal. *J. Aerosol Sci.* 30, S1, S783-S784 (Abstract of the 1999 Europ. Aerosol Conf., Prague, 6-10 September) (1999).

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

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

Part time: Ji. Čermák

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. 21]

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. 2, 3, 6, 7, 13-15]

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. 8, 11, 15]

Research and identification of sources of heavy metal air pollution

(K. Svoboda, supported by the Ministry of Environment of Czech Republic, Project V&V No. 520/1/97)

Investigation of present sources, types and time trends in heavy metal air pollution in Czech Republic, suggestions for emission control, analysis and measures for reduction of heavy metal emissions have been performed. Czech air pollution law/policy/norms were analysed and compared with the law/policy/norms of EU and suggestions were given to

improve the national law/norms toward the compatibility with the law/norms of EU. [Refs. 19, 20, 26]

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. A 4072801)

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, 5, 16-18]

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. 16-18, 22, 25]

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: DECHEMA, Würzburg, Germany

K. Svoboda: Taejon University, Taejon, KAIST Taejon and Kon-Kuk University Seoul, Korea

K. Svoboda: Tallinn Technical University, Tallinn, Estonia

Visitors

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

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

F. Sowa, A. Papamichalis: DMT Essen, Germany

J. Murani: VUEZ (Research Institute for Energetics), Levice, Slovakia

Publications

Papers

1. Čermák Ji., Svoboda K., Trnka O.: Jednoduchý model tvorby emisí NO pro spalování kapalných paliv ve fluidní vrstvě za zvýšeného tlaku. (Czech) A simple model for NO emissions in pressurized fluidized bed combustion of liquid fuels. *Ropa a Uhlí* 41, 33-36 (1999).
2. Hartman M., Trnka O., Svoboda K.: Potential of calcium oxide for removal of hydrogen sulphide and carbonyl sulphide from coal gas. *Acta Montana Ser. B*, 112(9), 5-18 (1999).
3. Hartman M., Svoboda K., Trnka O.: Effect of water vapour on the equilibrium between CaO and COS in coal gas. *Collect. Czech. Chem. Commun.* 64(1), 157-167 (1999).
4. Smolík J., Schwarz J., Veselý V., Sýkorová I., Kučera J., Havránek V.: Characterization of solid emissions from atmospheric fluidized-bed combustion of two Czech lignites. *Environ. Sci. Technol.* 33(20), 3543-3551 (1999).
5. Čermák Ji., Svoboda K., Hartman M.: Interferences by measurement of N₂O in flue gases with IR analysers and possibility of improvement of the measurement. *Chem. Pap.* (in press).
6. Hartman M., Trnka O., Svoboda K.: Fluidization characteristics of dolomite and calcined dolomite particles. *Chem. Eng. Sci.* (in press).
7. Hartman M., Trnka O., Svoboda K.: Essential factors in removing carbonyl sulphide from coal gas with lime and limestone. *Chem. Papers* (in press).
8. Hartman M., Trnka O., Veselý V., Svoboda K.: Thermal dehydration of the sodium carbonate hydrates. *Collect. Czech. Chem. Commun.* (in press).
9. Kučera J., Havránek V., Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Šantroch J.: INAA and PIXE of atmospheric and combustion aerosols. *Biol. Trace Element Res.* (in press).
10. 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.* (in press).
11. Trnka O., Veselý V., Hartman M., Beran Z.: Identification of the state of a fluidized bed by means of pressure fluctuations. *AIChE J.* (in press).
12. Veselý V., Hartman M., Svoboda K., Trnka O.: Spalování kapalných paliv ve fluidní vrstvě. (Czech) Incineration of liquid waste in fluidized bed. *Chem. Listy* (in press).

Review papers

13. Hartman M., Svoboda K., Trnka O., Veselý V.: Odsiřování horkého generátorového plynu tuhými sorbenty. (Czech) Removal of sulphur from hot coal gas. *Chem. Listy* 93, 99-106 (1999).
14. Hartman M., Svoboda K., Trnka O., Veselý V.: Síra při zplyňování uhlí. (Czech) Sulphur at coal gasification. *Chem. Listy* 93, 315-319 (1999).
15. Hartman M., Svoboda K., Trnka O., Beran Z.: Reaktory s cirkulující fluidní vrstvou. (Czech) Reactors with the circulating fluidized bed. *Chem. Listy* 93, 788-793 (1999).

16. Svoboda K., Hartman M., Čermák Ji.: Combustion processes - solid and liquid charring fuels. *Acta Montana, Ser. B*, 112(9), 55-79 (1999).
17. Svoboda K., Čermák Ji., Trnka O.: Chemistry and emissions of nitrogen oxides (NO, NO₂, N₂O) in combustion of solid fuels - heterogeneous reactions I. (NO + NO₂). *Chem. Pap.* (in press).
18. Svoboda K., Čermák Ji., Hartman M.: Chemistry and emissions of nitrogen oxides (NO, NO₂, N₂O) in combustion of solid fuels - heterogeneous reaction II. (NO₂). *Chem. Pap.* (in press).

Monographs

19. Svoboda K., Roček J., Čermák Ji.: Možnosti odlučování submikronových částic prachu z odpadních plynů a spalin. (Czech) Possibilities of removal of submicron dust particles from flue and waste gases. *Skripta pro postgraduální studium VŠCHT Praha*, 63 pp. (1999).
20. Svoboda K., Kepák F.: Energetika a životní prostředí. (Czech) Energetics and protection of environment. *Universita J. E. Purkyně, Fakulta životního prostředí*, pp. 270, Ústí nad Labem (1999).

Czech patents

21. 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

22. Čermák Ji., Svoboda K., Hartman M.: Interferences in measurement of N₂O in flue gases with IR analysers and possibility of improvement of the measurement. *26th International Conference SSChE, Proceedings*, p. 132, Jasná, Slovakia, 24-28 May (1999).
23. Punčochář M., Veselý V.: The reduction of POP emissions by using of sulphur additives. *26th International Conference SSChE, Proceedings*, p. 134, Jasná, Slovakia, 24-28 May (1999).
24. Smolík J., Schwarz J., Veselý V., Punčochář M., Kugler J., Sýkorová I., Havránek V.: Composition of particulate emissions from fluidised bed combustion of charcoal. *J. Aerosol Sci.* 30, S1, S783-S784 (Abstract of the 1999 Europ. Aerosol Conf., Praha, 6-10 September) (1999).
25. Svoboda K., Hartman M., Čermák Ji.: Pilot plant apparatus for pressurized fluidized bed combustion and gasification. *International Conference on the Ecological Use of Coal in the Energy sector "Clean Coal 2000", Book of Abstracts*. pp. 89-90, Praha, 31 May-3 June (1999).
26. Svoboda K., Heppner P., Hartman M., Čermák Ji.: Emission characteristics of selected Czech personal automobiles in typical driving regimes. *26th International Conference SSChE, Proceedings*, p. 80, Jasná, Slovakia, 24-28 May (1999).

Laser Chemistry Group

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

Part time: M. Jakoubková, J. Vítek

PhD students: K. Jursíková

Fields of research

- Laser induced chemistry
- Laser induced chemical vapour deposition of novel polymeric and Si-based materials
- Atmospheric chemistry: studies on reactions of ozone with olefinic pollutants and on laser-induced homogeneous decomposition of secondary ozonides
- Laser-induced polymerization in the gas phase
- Laser-induced photolysis of organosilicon, organoselenium and organotellurium compounds

Research projects

Studies of atmospheric chemistry and air pollution

(J. Pola, supported by GA CR, grant No. 104/96/0472)

Studies on the gas-phase low-temperature ozonolysis of alkenes provided the first experimental evidence of the formation of secondary ozonides in the gas phase and revealed that the stereospecificity for the conversion of *trans*-RHC=CHR olefins to *trans*-secondary ozonides in the gas phase is similar to that observed earlier in solution [Ref 1]. Studies on the gas-phase ozonolysis of trimethylsilylethenes in the gas phase shown that the ester channel of decomposition of the Criegee intermediate takes place exclusively via migration of trimethylsilyl group [Ref 2]. Studies on low-temperature ozonolysis of trimethylsilylethenes demonstrated feasibility of migrations of trimethylsilyl group in a dioxygen-centered diradical produced via homolysis of the O-O bond in the primary ozonide. These results provide the first evidence on the non-concerted decomposition of the primary ozonides.

Laser induced decomposition of hydridodisiloxanes

(J. Pola, supported by GA ASCR, grant No. A 4072806)

IR laser induced gas-phase and liquid-phase decompositions of various polyhydridodisiloxanes have been studied with the aim to reveal their suitability for production of novel silicon-based materials. The examination of CO₂ laser-induced graphite-photosensitized decomposition of 1,3-diphenyldisiloxane was revealed as the first example of silanone extrusion from linear-chain disiloxanes affording a blend of poly(phenylsiloxanes) [Ref 3]. IR laser induced homogeneous decomposition of disiloxane was described as dominated by elimination and polymerization of transient silanone. This process represents a convenient chemical vapour deposition of the yet unreported poly(hydridosiloxane) films [Ref 4]. UV laser photolysis of disiloxane proceeds as dehydrogenation and yields novel hydrogenated Si₂O phases [Ref 5]. UV laser photolysis of trimethyl(vinylxy)silane affords

polysiloxane films via cleavage of all but Si-O bonds of the precursor [Ref 6]. UV laser photolysis of 1,3-dimethyldisiloxane was revealed as a process yielding ultrafine hydrogenated silicone powders. These materials are potential precursors of novel organosilicon macromolecules with O-containing functional groups.

Laser induced synthesis of novel polymers

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

ArF laser photolysis of gaseous ethynyltrimethylsilane allows a controlled polymerization at the triple bond and represents a unique photopolymerization in the absence of photo-initiators, which is suitable for chemical vapour deposition of solid poly(trimethylsilyl-hydrocarbon) films [Refs. 7, 8]. 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)

Excimer laser photolysis of dialkyltelluriums and tellurophene in n-hexane affords nanosized Te and Te/C particles in which the Te/C ratio depends on the structure of the organotellurium precursor [Ref 9]. UV 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. UV laser photolysis of silacyclopent-3-ene proceeds as a clean extrusion of silylene and yields butadiene. In this process, the silylene self-polymerization is precluded by concurrently occurring photolysis of butadiene [Ref 10].

IR and UV laser induced photochemistry of disilanes for chemical vapour deposition of Si/C/H phases and chemical liquid deposition of polyhydrosilanes

(J. Pola, supported by Ministry of Education, grant No. ME225)

Studies on the use of single tailored organosilicon precursors for chemical vapour deposition of polycarbosilanes and silicon carbide has been continuing. It has been revealed that tert-butylsilane decomposes by IR laser radiation via elimination of isobutene and affords chemical vapour deposition of Si/C/H coatings [Ref 11].

Laser induced decomposition of hydrosiloxanes

(J. Pola, NATO collaborative research grant)

Infrared multiphoton decomposition of 1,3-dimethyldisiloxane has been demonstrated to yield nano-structured methyl(hydrido)silicone phase, a potential precursor to Si/C/O glasses and novel polymers with functional groups attached to silicon atom.

Studies on adsorption and reaction of ammonia and propylamines on alumina

(A. Galíková)

Kinetic studies of adsorption and reaction of propylamines on alumina using the Cahn recording microbalances revealed that the explaining of the so-called stop effect requires the assumption on blocking of the adsorption centers by the reaction products [Ref 12]. A study of adsorption of ammonia and of propylene has been therefore undertaken [Ref 13].

International co-operations

Bhabha Atomic Research Center, Bombay, India: Laser generation/detection of silicon-containing transients
Brandeis University, Waltham, USA: IR laser photosensitized isomerization of allene
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 alkylsilanes
Universität-GH, Wuppertal, Germany: Elusive silicon species for novel materials
University of Crete, Heraklion, Greece: Infrared multiphoton photolysis of disiloxanes

Visits abroad

J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (5 months)
J. Pola: Bergische Universität, Wuppertal, Germany (1 week)
J. Kupčík: Crete University, Heraklion, Greece (6 weeks)
M. Jakoubková: Instituto de Estructura de la Materia, CSIC Madrid, Spain (1 week)
K. Jursíková: Technical University, Graz, Austria: Laser chemistry of alkylsilanes (1 week)
K. Jursíková: Instituto de Estructura de la Materia, CSIC Madrid, Spain (1 week)
V. Dřínek: Technical University, Graz, Austria (1 week)
J. Pola: Crete University, Heraklion, Greece (2 weeks)

Visitors

A. Ouchi: Institute of Materials and Chemical Research, Tsukuba, Japan
K. Hassler: Technical University, Graz, Austria
S. Graschy: Technical University, Graz, Austria
Y. Koga: Institute of Materials and Chemical Research, Tsukuba, Japan
P. Papagiannakopoulos: Crete University, Heraklion, Greece
L. Tumanova: Institute of spectroscopy, Troitsk near Moscow, Russia
L. Diaz: Instituto de Estructura de la Materia, CSIC Madrid, Spain

Publications

Papers

1. Fajgar R., Vitek J., Haas Y., Pola J.: Formation of secondary ozonides in the gas phase low-temperature ozonation of primary and secondary alkenes. *J. Chem. Soc., Perkin 2*, 239-248 (1999).
2. Fajgar R., Pola J.: Trimethylsilyl group migration in Crigee intermediate in gas-phase ozonolysis of trimethylsilyl ethene. *Tetrahedron Lett.* (in press).

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6. Ouchi A., Koga Y., Bastl Z., Pola J.: UV-laser-induced photolysis of trimethyl(vinyl-oxy)silane for chemical vapour deposition of polysiloxane films. *Appl. Organometal. Chem.* 13, 643-647 (1999).
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8. Pola J., Urbanová M., Bastl Z., Šubrt Z., Ouchi A., Morita H.: Laser-induced formation of polymers from unsaturated (organyl)trimethylsilanes in the gas phase. *Polymer* (in press).
9. Ouchi A., Yamamoto K., Koga Y., Pola J.: Deposition of nanostructured Te and Te/C particles by excimer laser-induced photolysis of organotelluriums in the liquid phase. *J. Mater. Chem.* 9, 563-566 (1999).
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11. Pola J., Víték J., Bastl Z., Fajgar R., Graschy S., Hassler K.: Infrared laser-induced decomposition of tert-butylsilane for chemical vapour deposition of Si/C/H phases. *Main Group Met. Chem.* 22(9), 545-552 (1999).
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15. 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)* (in press).
16. Pola J.: IR and UV laser-induced decomposition of organosilanes for CVD of Si/C/H phases. *Res. Chem. Intermed.* 25(4), 351-366 (1999).

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19. Pola J.: Laser induced chemical vapour deposition of novel polymeric films. 2nd SAKEN International Symposium on Chemical and Physical Perspective for Molecular Devices, Proceedings pp. 142-149, Osaka University, Japan, 26-27 January (1999).

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Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

Applied research

- Analytical services to the research departments of ICPF

Research projects

Steric effects in NMR spectroscopy

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

Results of the above-mentioned project dealing with steric effects in ^{29}Si NMR are being extended to other fields of NMR to investigate the steric effects in general. [Refs. 3, 4, 9, 15]

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. [Ref. 16]

International co-operations

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

Catholic University of Leuven, Leuven, Belgium: NMR in medicinal chemistry

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"

R. Řeřicha: PICT, postgraduate course "Chemical Spectroscopy"

Publications

Papers

1. Balcar H., Sedláček J., Vohlídal J., Zedník J., Blechta V.: Schiff's base pendant groups by polymerization of benzylidene-ring-substituted N-benzylidene-4-ethynylanilines with Rh-based catalysts. *Macromol. Chem. Phys.* 200, 2591-2596 (1999).
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4. Schraml J., Kvíčalová M., Soukupová L., Blechta V., Exner O.: Silylation of substituted benzhydroxamic acids: NMR spectra (^{13}C , ^{15}N and ^{29}Si) and structure of tert-butyltrimethylsilyl derivatives. *J. Phys. Org. Chem.* 12, 668-674 (1999).
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11. Auerová K., Čermák Jan, Nguyen H. T. T., Blechta V.: The synthesis of metal complexes with cyclopentadienyl ligands containing perfluoroalkyl ponytails. XXXIst Symposium on Catalysis, p. Po18, Prague, 1-2 November (1999).
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15. Schraml J.: Derivates of hydroxamic acids. XIIIth FECHEM Conference on Organometallic Chemistry 1999, Book of Abstracts, p. 38, Lisboa, Portugal, 29 August-3 September (1999).
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Miscellaneous

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