

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 1998

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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 10)
Department of Catalysis and Reaction Engineering	(page 17)
Department of Multiphase Reactors	(page 23)
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STAFF

(31 December 1998)

Category	Number of Employees
Research □	116 □
Technical □	25 □
Administrative □	18 □
Services □	18 □

BUDGET 1998

(in million Kč; 32 Kč = 1 US\$, approx.)

Institutional support from National Budget	40
Research funds from Grant Agencies	17
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: M. Chačaturjan, V. Staněk, H. Vychodilová
Technical staff: A. Kadlecová, D. Karfík, R. Kloudová, R. Petříčkovič, D. Vlček
PhD students: 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
- Dynamic behaviour of two-phase gas-liquid flow in packed columns and reactors
- Amine extraction of hydroxycarboxylic acids; extraction and refining of phenols from coal tars; liquid-liquid extraction of heavy metals
- Supercritical fluid extraction of essential oils; 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
- Refining of plant extracts
- Preparation of corundum support for ceramic membranes
- Evaluation of commercial ion exchanger catalysts for bisphenol A synthesis
- Purification of a mixture of solids using supercritical CO₂ as a solvent

Research projects

Composite ceramic membranes

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

Corundum membrane support of very good mechanical resistance was prepared. The preparation method makes possible to control pore size and porosity of the product. Successfully was finished the development of a pressure coating method for producing of microfiltration layers and their thermal treatment.

Polymer-supported ligands for ecological problems

(K. Jeřábek, joint project with Weizmann Institute of Science, Rehovot, Israel; supported by the Agency for International Development, Washington, USA, grant No. TA-MOU-C13-085)

Solvent impregnated resins prepared by supporting various dialkylphosphoric acids on functionalized polymer carriers were investigated [Refs. 3, 22]. Active substance is absorbed on these supports into the skeleton of the relatively hydrophilic polymer carrier. For separation of metal ions from aqueous solutions, the resulting morphology is much more advantageous than that of the more conventional solvent impregnated resins prepared on the basis of inert hydrophobic polymer supports [Ref. 28].

Molecular accessibility of microporous matrixes

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

The macromolecular structure and chemical accessibility of polymer supported metal catalysts were studied. Inverse steric exclusion chromatography-derived description of the working-state morphology of polymer catalysts was confronted with catalytic experiments. [Refs. 1, 2, 16]

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)

In the starting period of this project, a method was developed for the investigation of residence time profiles of gas in the column apparatus. The method is based on injection of helium into the gas stream and continuous measurements of thermal conductivity of the output gas. [Refs. 8, 15, 20, 21]

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. 4, 7, 23, 24]

Extraction of molybdenum and tungsten by tertiary amines

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

Equilibria in systems aqueous solution of sulfuric acid - solution of trioctylamine in the mixture of dearomatized kerosene and octanol were measured, and a model describing the effect of the amine concentration in the solvent was formulated. [Refs. 9, 25]

Solubilities in supercritical fluids - measurement and modelling

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

Solubility of four solutes (limonene, beta-carotene, trans-ferulic acid and glycerol) in carbon dioxide was measured by dynamic method and the phase equilibrium was simulated by a thermodynamic model. Preliminary experiments and modelling of these solutes in CO₂ with entrainer as a third component were performed [Refs. 6, 17, 18]. Extraction of essential oils from peppermint and thyme with supercritical carbon dioxide was studied and compared with hydrodistillation [12, 13].

International cooperations

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 Skopje, Macedonia: Extraction of hydroxycarboxylic acids, supercritical fluid extraction of natural products
Institute of Chemical Engineering, Sofia, Bulgaria: Separation of heavy metals from aqueous solutions using amine extractants.
Otto von Guericke University of Magdeburg, FRG: Determination of porous structure of ceramic membranes
Korean Research Institute of Chemical Technology, Taejon, South Korea: Diffusion of binary mixtures in polymeric membranes during the pervaporation,
Hiroshima University, Japan: Pervaporation on ceramic membranes

Visits abroad

A. Heyberger: University of Durban, AECI, South Africa
K. Jeřábek: University of Padua, Italy; The Weizmann Institute of Science, Rehovot, Israel; Universitat Politecnica de Catalunya, Universitat Autònoma de Barcelona, Universitat Barcelona, Barcelona, Spain
V. Jiříčný: University of California, Berkeley, USA
H. Sovová: Institute of Chemical Engineering, Sofia, Bulgaria, University of Skopje, Macedonia
P. Uchytíl: Hiroshima University, Japan (2 months); Otto von Guericke University of Magdeburg, FRG;

Visitors

A. D'Archivio, B. Corain, University of L'Aquila, Italy
A. Biffis, M. Zecca, University of Padua, Italy
I. Mishonov, Institute of Chemical Engineering, Sofia, Bulgaria

Teaching

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

Publications

Papers

1. Jeřábek K., Prokop Z.: Possibilities of decreasing absorption of water in ion-exchanger catalysts. *Collect. Czech. Chem. Commun.* 63(11), 1907-1914 (1998).
2. Králík M., Fišera R., Zecca M., Archivio A., Galantini C., Jeřábek K., Corain B.: Modelling of the deactivation of polymer-supported palladium catalysts in the hydrogenation of 4-nitro-toluene. *Collect. Czech. Chem. Commun.* 63 (7), 1074-1088 (1998).
3. Strikovski A. G., Warshawski A., Hanková L., Jeřábek K.: Morphology of solvent-impregnated resins based on reactive supports. *Acta Polymerica* 49, 600-605 (1998).
4. Tomovska R., Poposka F., Volaufová E., Heyberger A., Procházka J.: Extraction of tartaric acid with trialkylamine. *Collect. Czech. Chem. Commun.* 63(3), 305-320 (1998).
5. Tuchlenski A., Uchytíl P., Seidel-Morgenstern A.: An experimental study of combined gas phase and surface diffusion in porous glass. *J. Membr. Sci.* 140, 165-184 (1998).
6. 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).
7. Poposka F., Procházka J., Tomovska R., Nikolovski K., Grizo A.: Extraction of tartaric acid from aqueous solutions with tri-iso-octylamine (HOSTAREX A 324). Equilibrium and kinetics. *Chem. Eng. Sci.* (in press).
8. Staněk V., Jakeš B., Svoboda P., Ondráček J., Jiříčný V.: Characteristics of pressure and liquid holdup overshoot following a sudden increase of gas flow. *Chem. Eng. J.* (in press).
9. Vachtová J., Heyberger A., Mrnka M., Procházka J.: Extraction of sulfuric acid with trialkylamine in a mixed diluent. *Ind. Eng. Chem. Res.* (in press).
10. Veverka L., Jeřábek K.: Mechanism of hypercrosslinking of chloromethylated S-DVB copolymers. *React. Func. Polym.* (in press).

Monographs

11. Svoboda K., Roček J., Čermák Jiří: Možnosti odlučování submikronových částic prachu z odpadních plynů a spalín. (Czech) Possibilities of removal of submicron dust particles from flue and waste gases. *Skripta pro postgraduální studium VŠCHT Praha*, 63 pp. (1999).

Conferences

12. Aleksovski S., Sovová H., Poposka F., Curapova B.: Supercritical fluid extraction as advanced method for extraction of essential oils from aromatic plants. 8th International Summer School for Chemical Engineering, p. 241, Sozopol, Bulgaria, 3-9 June (1998).
13. Aleksovski S., Sovová H., Poposka F., Curapova B.: Supercritical fluid extraction of essential oils from peppermint and wild thyme and its comparison with hydrodistillation. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 4, p. 118, Praha, 23-28 August (1998).
14. Asaeda M., Uchytíl P., Tsuru T., Yoshioka T., Ootani M., Nakamura N.: Pervaporation of methanol-MTBE mixture by porous silica-zirconia (10%) membranes. *Proceedings of the Fifth International Conference on Inorganic Membranes*, pp. 322-325, Nagoya, Japan, 22-26 June (1998).
15. Jakeš B., Staněk V., Ondráček J., Svoboda P., Jiříčný V.: Použití heliové sondy pro studium dynamiky náplňové kolony. (Czech) Application of He-probe for the study of the dynamics of packed bed. 3. Vědecko-technická konference "Řízení procesů'98", Kouty nad Desnou, 7-10 Juni (1998).

16. Jeřábek K.: Inverse steric exclusion chromatography (isec): a powerful tool in polymer structure characterization. 8th Int. Conference on Polymer-Based Technology POC'98, p. 47, Ma'ale, Hachamisha, Izrael, 28 June-2 July (1998).
17. Sovová H., Stateva R. P.: Solubility of liquids in supercritical CO₂ with entrainers. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 4, p. 26, Praha, 23-28 August (1998).
18. Sovová H., Stateva R. P.: Increasing solubility in dense CO₂ with entrainers.. 8th International Summer School for Chemical Engineering, pp. 173-174, Sozopol, Bulgaria, 3-9 June (1998).
19. Staněk V., Hanika J.: Flow transients and gas residence time measurement in packed columns under two-phase counter-current flow. 13th International Congress of Chemical and Process Engineering CHISA'98, Praha, 23-28 August (1998).
20. Staněk V., Jakeš B., Svoboda P., Ondráček J., Jiříčný V.: Přejížděcí stavy hydrodynamiky dvoufázového toku v náplňové koloně. (Czech) Transient states of the hydrodynamics of two-phase flow in a packed bed. 3. Vědecko-technická konference "Řízení procesů '98", Kouty nad Desnou, 7-10 Juni (1998).
21. Strikovski A., Jeřábek K., Warshawsky A.: Novel polymeric acid-base-coupled extractants. 8th International Conference on Polymer-Based Technology POC'98, p. 133, Ma'ale Hachamisha, Izrael, 28 June-2 July (1998).
22. Tomovska R., Poposka F., Heyberger A., Procházka J.: pH-dependence of tartaric acid extraction. 13th International Congress of Chemical and Process Engineering CHISA'98, Abstracts P3, p. 450, Praha, 23-28 August (1998).
23. Tomovska R., Volaufová E.: Extrakce kyseliny vinné trialkylaminem. (Czech) Extraction of tartaric acid with trialkylamine. 25. konferencia SSCHI, Zborník p. 96, Jasná, Slovakia, 25-29 May (1998).
24. Vachtová J., Mrnka M., Heyberger A., Procházka J.: Extraction of sulphuric acid with trialkylamine in a mixed diluent. 13th International Congress of Chemical and Process Engineering CHISA'98, Abstracts P3, p. 378, Praha, 23-28 August (1998).
25. Veverka P., Jeřábek K.: Mechanism of hypercrosslinking of chloromethylated S-DVB copolymers. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 4, p. 191, Praha, 23-28 August (1998).
26. Veverka P., Jeřábek K.: Mechanism of hypercrosslinking of chloromethylated S-DVB copolymers. 8th International Conference on Polymer-Based Technology POC'98, p. 140, Ma'ale Hachamisha, Izrael, 28 June-2 July (1998).
27. Warshawsky A., Strikovski A., Jeřábek K.: Solvent impregnated resins (SIR): Fundamental and applied aspects. Research Workshop: Chemical, Structural and Biochemical Applications of Supramolecular Systems, Tel-Aviv, Israel, 3-7 January (1998).

E. Hála Laboratory of Thermodynamics

Head: I. Wichterle
Deputy: K. Aim
Research staff: J. Kolafa, J. Linek, M. Lísal, I. Nezbeda, J. Pavlíček, M. Strnad, Z. Wagner
Visiting: M. Teodorescu
Part time: T. Boublík
Technical staff: S. Bernatová, Š. Psutka
PhD students: O. Dahmani, É. Kovács, M. Předota, 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)

New data for the two-centre Lennard–Jones dipolar model fluid along the vapour-liquid coexistence region have been generated by molecular simulations for selected elongations and wide range of dipole moments. The accuracy of data obtained by different methodologies has been assessed and a benchmark data set established. A relatively simple anisotropic interaction potential has been successfully applied to calculating the state and phase properties of chlorine. The study on developing and testing analytical equations of state for systems containing associating fluids based on primitive model of association has continued. [Refs. 14, 18-22, 32, 33, 37, 39]

Experimental thermodynamics of organic compounds and their aqueous solutions at extreme conditions: application to environmental and energetic systems

(K. Aim, joint project with PICT; supported by GA CR, grant No. 203/96/1162)

Accurate data on temperature dependences of the vapour pressures of 2-chlorophenol, 2-chlorotoluene, 4-chlorotoluene, perhydroacenaphthene, perhydrophenanthrene, 2-pentanol, 3-pentanol, 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and 3-methyl-2-butanol have been measured by high precision comparative ebulliometry over the approximate pressure range of 5 to 100 kPa. [Refs. 7, 13, 28, 46, 47]

Equilibrium behaviour of fluids constituted of anisotropic molecules

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

The potentialities of the full second-order perturbation theory for fluids constituted of anisotropic molecules have been further investigated. The ability of the theory to represent the excess properties of mixing in binary systems of linear alkanes (differing in chain length) modelled as rods interacting by way of Kihara potential is very good. Excellent results are obtained for fluids made up of relatively small (i.e. rigid) molecules, especially if temperature dependence of the interaction potential parameters is somewhat relaxed. Excess volume data have been determined experimentally for a series of binary systems of the type linear alkane (C_5 or C_6) plus chlorinated hydrocarbon (C_2 to C_6). An apparatus for the measurement of densities of liquid mixtures at high pressures has been assembled and tested. [Refs. 10, 11, 17, 26, 34-36, 44]

General phase behavior of binary fluid mixtures: theory and application of global phase diagrams

(J. Kolafa, supported by ICPF ASCR)

The aim of the project is to determine global phase diagrams of binary fluid mixtures and to use them for predicting types of pressure–temperature–composition phase behaviour. We focused on the mixture of attractive hard spheres with different energy combining rules where new azeotropic phenomena at low temperatures were found. In addition, the global phase diagram of a mixture of water and n-alkanols described by the SAFT equation of state was studied. [Refs. 1, 25]

Pressure–volume–temperature behaviour of liquids and liquid mixtures

(J. Linek, supported by ICPF ASCR)

Apparatus for measuring P-V-T relations of liquids and liquid mixtures at elevated pressures and temperatures was designed and tested. Densities of liquids and excess volumes of a number of liquid mixture systems were determined by a DMA 58 Paar densimeter at 298.15 K partly to complement the vapour–liquid equilibrium data, partly to study the interactions between the corresponding molecules. [Refs. 11, 12, 17, 35, 36, 49]

Molecular modelling of aqueous solutions of electrolytes

(I. Nezbeda, supported by GA ASCR, grant No. A4072607)

To study aqueous solutions of electrolytes on a molecular level, a molecular model of water must be developed first. A family of a new class of primitive models of water, the so-called extended primitive models, has been developed and studied both theoretically and by means of computer simulations. [Refs. 5, 9, 42]

Binary mixtures with associating components: molecular and phenomenological theories and experiment

(I. Nezbeda, joint project with PICT; supported by GA CR, grant No. 203/96/0585)

A new family of primitive models of water, the so-called extended primitive models, has been developed and studied both theoretically and by means of computer simulations. Simultaneously, for further applications, a software for the determination of the phase behaviour and global phase diagrams has been developed. [Refs. 1, 5, 6, 9, 25, 33, 41, 42]

Solubility of hydrophobic compounds in water: theoretical and experimental study

(I. Nezbeda, joint project with PICT; supported by GA CR, grant No. 203/96/0494)

In the focus of investigations there have been various methods for the determination of the chemical potential in dense systems and general problems of phase behaviour of systems with an associating component. A new method of the numerical integration of equations of motion in molecular dynamics has been developed. Hydrophobic hydration has been studied at the level of primitive models. [Refs. 8, 16, 27, 29, 43, 48]

Vapour-liquid equilibrium (modelling and experiment)

(I. Wichterle, joint project with PICT; supported by GA CR, grant No. 104/96/0571)

Experiments: Systematic determination of vapour-liquid equilibria and excess molar volumes in series of model binary and ternary systems (containing ether + alcohol + hydrocarbon) have been carried out. Data processing: New group contributions for C=O/Cl interaction were evaluated for the DISQUAC prediction methods. Data base: Vapour-liquid equilibrium data bibliography was supplemented by the end of 1997 and published as the book and as the software. [Refs. 4, 10-12, 15, 30, 49-53]

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 preliminary experimental tests have been carried out. The Monte Carlo simulations have been successfully performed for the simple reaction $\text{Br}_2 + \text{Cl}_2 \rightleftharpoons 2\text{BrCl}$. [Ref. 23, 40]

International cooperations

DICAMP, University of Trieste, Trieste, Italy: Phase equilibria for supercritical fluid technology
University of Guelph, Guelph, Canada: Statistical mechanics of liquids – equilibria on molecular level

Universität Erlangen, Erlangen, FRG: Equation of state and chemical equilibrium

Sonderforschungsbereich, Universität Leipzig, Leipzig, FRG: Fluid in confined geometry

University of Odense, Odense, Denmark: PROSIS – Protein simulation software

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

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

University of Oklahoma, Norman, Oklahoma, USA: Molecular theories of solutions of electrolytes

National Science Foundation with University of Oklahoma, Norman, USA: Water cleanup using oxidation

Visits abroad

- K. Aim: Korea University, Seoul National University, Sogang University, Seoul; Korean Advanced Institute of Science and Technology, Taejon, South Korea
J. Kolafa: University of Odense, Odense, Denmark (1 month)
I. Nezbeda: Universität Leipzig, Leipzig, FRG; Agriculture University, Wien, Austria
J. Pavlíček: Universität Erlangen, Erlangen, FRG (12 months)

Visitors

- A. Dahmani: Université de Science et Technologie, Alger, Algeria (1 month)
M. Teodorescu: Romanian Academy, Bucharest, Romania (4 months)
W. R. Smith, D. Drummond: University of Guelph, Guelph, Canada
H. Vörtler: Universität Leipzig, Leipzig, FRG

Teaching

- K. Aim: PICT, postgraduate courses "Applied statistical analysis and data processing"
T. Boublík: CU, courses "Basic physical chemistry", "Advanced chemical thermodynamics", and "Statistical thermodynamics"
J. Kolafa: CU, course: "Computer simulations"
I. Nezbeda: Purkyně University, courses: "Analytical mechanics", "Introduction to computer simulations", "Mathematics for Physicists", "Thermodynamics and Statistical Physics"

Publications

Papers

1. Kolafa J., Nezbeda I., Pavlíček J., Smith W. R.: Global phase diagrams of model and real binary fluid mixtures: Lorentz-Berthelot mixture of attractive hard spheres. *Fluid Phase Equilib.* 146, 103-121 (1998).
2. Kotrla M., Předota M., Slanina F.: Kinetic roughening and phase ordering in the two-components growth model. *Surface Sci.* 402-404 (1998).
3. Kolafa J., Ratner M.: Oligomers of poly(ethylene oxide): molecular dynamics with a polarizable force field. *Molec. Simulations* 21, 1-26 (1998).
4. Linek J., Wichterle I.: Isothermal vapor-liquid equilibria at temperatures from 320. 00 K to 340. 00 K and densities at the temperature 298. 15 K for ethyl propanoate + butyl methyl ether or tert-butyl methyl ether. *ELDATA J.* 3, 235-242 (1997); published (1998).
5. Nezbeda I.: Structure of water: short-ranged versus long-ranged forces. *Czech. J. Phys.* 48(1), 117-122 (1998).
6. Předota M., Nezbeda I., Kalyuzhnyi Yu. V.: Fluid of pseudo-hard bodies. II. Reference models for water, methanol and ammonia. *Molec. Phys.* 94(6), 937-948 (1998).

7. Roháč V., Růžička V., Růžička K., Aim K.: Measurement of saturated vapor pressure above liquid phase for dichlorobenzenes and 1, 2, 4-trichlorobenzene. *J. Chem. Eng. Data* 43, 770-775 (1998).
8. Smith W. R., Nezbeda I., Strnad M., Tříska B., Labík S., Malijevský A.: Generalized thermodynamic perturbation theory for polyatomic fluid mixtures. I. Formulation and results for chemical potentials. *J. Chem. Phys.* 109(3), 1052-1069 (1998).
9. Strnad M., Nezbeda I.: Extended primitive models of water revisited. *Molec. Phys.* 93(1), 25-30 (1998).
10. Teodorescu M., Aim K., Wichterle I.: Isothermal vapour-liquid equilibria for pentan-3-one + 1, 4-dichlorobutane, + trichloromethane, + 1, 1, 1-trichloroethane, + 1, 1, 2, 2-tetrachloroethane binary mixtures. *Fluid Phase Equilib.* 147, 215-228 (1998).
11. Teodorescu M., Linek J.: Densities and excess volumes of pentan-3-one + 1, 2-dichloroethane, + 1, 3-dichloropropane, + 1, 4-dichlorobutane, + trichloromethane, + 1, 1, 1-trichloroethane, + 1, 1, 2, 2-tetrachloroethane binary mixtures at 298. 15 K. *Fluid Phase Equilib.* 146, 155-160 (1998).
12. Teodorescu M., Linek J., Wichterle I.: Isothermal vapour-liquid equilibria and densities for the 5-chloropentan-2-one + n-hexane, + toluene and + ethylbenzene binary mixtures. *Fluid Phase Equilib.* 149, 127-138 (1998).
13. Aim K.: Vapor pressures of 2-chlorotoluene and 4-chlorotoluene and relative volatility in their binary system. *Thermochim. Acta* (in press).
14. Aim K.: On practical equations of state for methanol based on molecular theory. *Fluid Phase Equilib.* (in press).
15. Dahmani O., Wichterle I.: HSE conformal solution theory with the Lennard-Jones (12-6) intermolecular potential. *Fluid Phase Equilib.* (in press).
16. 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).
17. Kovács É., Linek J.: Densities and excess volumes of heptane with 1-chloropropane, 1-chlorobutane, 1-chloropentane, and 1-chlorohexane binary mixtures at 298. 15 K. *Collect. Czech. Chem. Commun.* (in press).
18. Lísal M., Aim K., Vacek V., Černý F.: Vapour-liquid equilibria of alternative refrigerants from a simple model fluid. *Acta Polytech.* (in press).
19. 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.* (in press).
20. Lísal M., Nezbeda I., Vörtler H. L.: Fluid-solid boundary of the compressed exp-6 fluids. *Fluid Phase Equilib.* (in press).
21. Lísal M., Nezbeda I.: Pure fluids of homo- and hetero-nuclear square-well diatomics. I. Computer simulation study. *Molec. Phys.* (in press).
22. Lísal M., Budinský R., Vacek V., Aim K.: Vapour-liquid equilibria of alternative refrigerants by molecular dynamics simulations. *Int. J. Thermophys.* (in press).
23. 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.* (in press).
24. Nezbeda I., Aim K.: A general method improving phase equilibrium calculations from pressure-explicit equations of state. *Fluid Phase Equilib.* (in press).
25. Nezbeda I., Pavlíček J., Kolafa J., Galindo A., Jackson G.: Global phase behavior of mixtures of water and n-alkanols. *Fluid Phase Equilib.* (in press).
26. Pavlíček J., Boublík T., Aim K.: Fluids of the Kihara molecules II. Binary mixtures of n-alkanes. *J. Phys. Chem.* (in press).

27. Předota M, Nezbeda I.: Hydrophobic hydration at the level of primitive models. *Mol. Phys.* (in press).
28. Roháč V., Musgrove J. E., Růžička K., Růžička V., Aim K., Záborský M.: Thermodynamic properties of dimethyl phthalate along vapour-liquid saturation curve. *J. Chem. Thermodyn.* (in press).
29. Strnad M., Nezbeda I.: Extended Gibbs ensemble: a set of Gibbs ensembles with a fluctuating particle. *Mol. Phys.* (in press).

Monographs

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33. Aim K., Kolafa J., Nezbeda I.: Equations of state based on primitive models of association and their applications to systems containing methanol. 8th International Conference on Properties and Phase Equilibria for Product and Process Design, Abstr. p. 51, Noordwijkerhout, The Netherlands, 26 April-1 May (1998).
34. Aim K., Pavlíček J.: Phase and state behavior of binary systems of hydrocarbons from the perturbation theory for anisotropic molecules. 15th International Conference on Thermodynamics, Book of Abstracts C1-10, Porto, Portugal, 26 July-1 August (1998).
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36. Kovács E., Linek J.: P-V-T relations of liquids and liquid mixtures at elevated temperatures and pressures. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 5, p. 20, Praha, 23-28 August (1998).
37. Lísal M., Aim K.: Prediction of thermodynamic properties of chlorine by molecular dynamics simulations with anisotropic interaction potential. 5th Asian Thermophysical Properties Conference ATPC'98, Proceedings, pp. 99-104, Seoul, Korea, 30 August-2 September (1998).
38. Lísal M., Nezbeda I.: Square-well diatomic fluids: computer simulation study. 5th Liblice Conference of the Statistical Mechanics of Liquid, Železná Ruda, Czech Republic, 7-12 June (1998).
39. Lísal M., Aim K.: Phase behavior of dipolar two-center Lennard-Jones fluid: Computer simulations and equation of state. 5th Liblice Conference on the Statistical Mechanics of Liquids, Poster No. 86, Železná Ruda, Czech Republic, 7-12 June (1998).
40. Lísal M., Nezbeda I., Smith W. R.: Reaction ensemble Monte Carlo simulation: phase equilibria in the reactive mixture of bromine and chlorine. 5th Liblice Conference on the Statistical Mechanics of Liquids, Železná Ruda, Czech Republic, 7-12 June (1998).
41. Nezbeda I., Pavlíček J., Kolafa J., Galindo A., Jackson G.: Global phase behavior of mixtures of water and n-alkanols. 8th International Conference on Properties and Phase

- Equilibria for Product and Process Design, Noordwijkerhout, The Netherlands, 26 April-1 May (1998).
42. Nezbeda I.: Simple models of association: from understanding to applications. EMLG Annual Meeting, Murrau, Austria, 10-16 September (1998).
 43. Nezbeda I., Předota M.: Hydrophobic hydration at the level of primitive models. 5th Liblice Conference on the Statistical Mechanics of Liquids, Železná Ruda, Czech Republic, 7-12 June (1998).
 44. Pavlíček J., Aim K.: Excess functions for binary mixtures of fluids of Kihara rod-like molecules differing in size. 5th Liblice Conference on the Statistical Mechanics of Liquids, Poster No. 102, Železná Ruda, Czech Republic, 7-12 June (1998).
 45. Předota M., Nezbeda I.: Fluids of pseudo-hard bodies: theory and experiment. 5th Liblice Conference on the Statistical Mechanics of Liquids, Železná Ruda, Czech Republic, 7-12 June (1998).
 46. Roháč V., Růžička V., Růžička K., Jose J., Aim K.: Thermodynamic properties of esters of phthalic acid at ambient temperatures. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 5, p. 15, Praha, 23-28 August (1998).
 47. Růžička V., Roháč V., Růžička K., Poledníček M., Aim K., Jose J., Zábanský M.: Recommended vapor and sublimation pressures and related thermal data for chlorobenzenes. 8th International Conference on Properties and Phase Equilibria for Product and Process Design, Abstr. p. 69, Noordwijkerhout, The Netherlands, 26 April-1 May (1998).
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 49. Teodorescu M., Linek J., Wichterle I.: Thermodynamic properties of binary 5-chloropentan-2-one + n-hexane, toluene and ethylbenzene mixtures. 15th International Conference on Chemical Thermodynamics, Book of Abstracts P1-8, Porto, Portugal, 26 July-1 August (1998).
 50. Teodorescu M., Wichterle I.: DISQUAC interaction parameters for C=O/Cl group in the pentan-3-one + chloroalkane mixtures. 15th International Conference on Thermodynamics, Book of Abstracts C1-25, Porto, Portugal, 26 July-1 August (1998).
 51. Wagner Z.: Využití gnostické teorie při zpracování fyzikálně-chemických dat. (Czech) Application of gnostic theory to analysis of physico-chemical data. 25. konferencia SSCHI, Zborník p. 49, Jasná, Slovakia, 25-29 May (1998).
 52. Wagner Z.: Estimation of interaction parameters of equations of state using object oriented method. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 5, p. 12, Praha, 23-28 August (1998).
 53. Wagner Z.: Application of gnostic theory to high-pressure vapour-liquid equilibrium and other physico-chemical data. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 4, p. 24, Praha, 23-28 August (1998).

Department of Catalysis and Reaction Engineering

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

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

Permeation of gases in porous solids

(O. Šolcová, supported by GA ASCR, grant No. 4072706)

A new permeation cell for study of gas flow through porous solids under pressure gradient was constructed. In this cell, both the steady-state as well as dynamic permeation processes can be followed. The response signals from the automated cell are fed to a PC for numerical processing. [Ref. 36]

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 countercurrently 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. 42-44]

Dynamics of the system: amines - aluminium oxide

(K. Klusáček, supported by ICPF ASCR)

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. [Refs. 15, 34]

Catalytic and adsorption processes for environmental pollution control - scientific network

(K. Klusáček, supported by grant PECO-Action, proposal No. 2872)

The objective of the project is to establish contacts among the scientists of the European countries engaged in the research and development of various techniques of chemical engineering oriented to the direct application in the environmental pollution control.

Sulphide hydrotreating catalysts: exploration of new active phases, supports and preparation methods

(M. Zdražil, supported by GA CR, grant No. 104/96/0573)

The activity of the Ir/Al₂O₃ catalysts was tested in parallel hydrodenitrogenation of pyridine and hydrodesulphurization of thiophene, and the effect of Ir dispersion and sulphur addition was evaluated. The Ir catalysts were more active than the conventional NiMo/Al₂O₃ sulphide system. [Refs. 13, 32]

Mo/alumina catalysts were modified by small amount of Ir below 1 wt. %. Depending on the way of preparation, some combinations possessed markedly higher HDN activity and HDN/HDS selectivity in comparison to monometallic systems.

Deposition of MoO₃ on alumina is accompanied by the consumption of OH groups of the support. Titration of catalysts with dimethylzinc permits a quantitative description of this process and the OH/Mo stoichiometry can be evaluated. This approach gives information about surface chemistry and calculation of molybdene coverage of the MoO₃/Al₂O₃ catalysts. [Refs. 45, 46]

The synergistic effect between Ni and W in activity of the Ni-W catalyst in parallel hydrodenitrogenation of pyridine and hydrodesulphurization of thiophene is accompanied by the characteristic shift of the hydrodenitrogenation/hydrodesulphurization selectivity to the hydrodesulphurization side. [Ref. 16]

New precursors of supported Mo catalysts

(Z. Vít, supported by ICPF ASCR)

Catalysts containing non-stoichiometric Mo oxides were prepared by the equilibrium adsorption on alumina and tested in hydrorefining reactions. Interaction of Mo compounds with alumina support is studied and compared with conventional MoO₃-alumina system.

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 high surface area MoO₃/MgO (200-300 m²g⁻¹) was prepared by the new method of the reaction of high surface area MgO with the slurry of ammonium heptamolybdate in methanol. The activity of the catalysts was tested in hydrodesulphurization of benzothiophene, and it was

found that it is comparable to the activity of the conventional $\text{MoO}_3/\text{Al}_2\text{O}_3$ catalyst. [Refs. 22, 40]

Catalytic combustion of volatile organic compounds

(K. Jirátová, supported by ICPF ASCR)

Combustion of ethanol over silica supported transition metal salts of phosphomolybdic acid was studied. Special attention was paid to the formation of the reaction intermediates (e.g., acetaldehyde) and to the effect of the way of catalyst preparation on its activity and selectivity. [Refs. 21, 39]

Chemical applications and theoretical interpretation of pair density matrices

(R. Ponec, supported by GA ASCR, grant No. A4072606)

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. [Refs. 7, 8, 26-28]

International cooperations

Analysis of the pair density matrix: University of Liverpool, Liverpool, UK; Universität Hannover, Hannover, FRG; 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

K. Jirátová: Universities of Hsinchu, Tainan, Taipei, Chung-li, Taiwan (2 weeks)

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

R. Ponec: University of Buenos Aires, Buenos Aires, Argentina (1 month)

Visitors

M. Bren, University of Maribor, Slovenia

A. Duben, University of Missouri, USA

N. Kostova, Institute of Catalysis, Sofia, Bulgaria

Teaching

K. Jirátová: 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" and "Applied catalysis"

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

K. Klusáček: PICT, postgraduate course "Nonstationary Methods in Heterogeneous Catalysis"

Publications

Papers

1. Amat L., Carbo-Dorca R., Ponec R.: A new classification for hydrophobicity. Molecular quantum similarity measures as alternatives to LogP. *J. Comput. Chem.* 14, 1575 (1998).
2. Bochicchio R., Ponec R., Lain L., Torre A.: On the physical meaning of bond indices from the population analysis of higher order densities. *J. Phys. Chem. A* 102, 7176 (1998).
3. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Dynamics of pressure build-up accompanying multicomponent gas transport in porous solids: inert gases. *Chem. Eng. J.* 70, 189-195 (1998).
4. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Dynamic gas transport in porous bidispersed alumina. *Collect. Czech. Chem. Commun.* 63(11), 1954-1962 (1998).
5. Hudec P., Smiešková A., Židek Z., Zúbek M., Schneider P., Kočířík M., Kozánková J.: Adsorption properties of ZSM-5 zeolites. *Collect. Czech. Chem. Commun.* 63, 141-153 (1998).
6. Ponec R.: Electron pairing and chemical bonds. Molecular structures from the analysis of pair densities and related quantities. *J. Match. Chem.* 23, 85 (1998).
7. Ponec R.: Similarity approach to chemical reactivity. Spin recoupling in chemical reactions. *Croat. Chem. Acta* 71, 501 (1998).
8. Ponec R.: Electron pairing and chemical bonds. Chemical bonds from the condition of minimum fluctuation of electron pair. *Int. J. Quantum Chem.* 69, 193-200 (1998).
9. Schneider P.: Effectiveness factor for a non-isothermal simple catalytic reaction with combined transport processes: Maxwell-Stefan approach. *Collect. Czech. Chem. Commun.* 63, 252-270 (1998).
10. Spojakina A. A., Kostova N. G., Jirátová K.: Effect of heteroatom on properties of the SiO₂-supported heteropolymolybdates. *Collect. Czech. Chem. Commun.* 63 (11), 1927-1937 (1998).
11. Zamlynyy V., Kubelková L., Babůrek E., Jirátová K., Nováková J.: Amination of cyclohexanol over metallosilicate based material. *Appl. Catal. A* 109, 119-125 (1998).
12. Amat L., Carbó-Dorca R., Ponec R.: Molecular quantum similarity measures as an alternative to log P values in QSAR studies. *J. Comput. Chem.* (in press).
13. Cinibulk J., Vít Z.: Hydrodenitrogenation of pyridine over alumina-supported iridium catalysts. *Appl. Catal.* (in press).
14. Fišer J., Gulková D., Zdražil M.: Hydrodesulphurization of benzothiophene over magnesia supported Ni, Mo and Ni-Mo sulphide catalysts prepared by non-aqueous impregnation: high activity and synergistic shift in selectivity to dihydrobenzothiophene. *Bulg. Chem. Commun.* (in press).
15. Galík A., Galíková A., Klusáček K.: Gravimetric transient response study of adsorption and reaction of propylamines on alumina. *Chem. Eng. Sci.* (in press).
16. Gulková E., 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.* (in press).
17. 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.* (in press).

18. Hudec P., Smiešková A., Židek Z., Zúbek M., Schneider P., Kočířík M., Kozánková J.: Adsorption properties of ZSM-5 zeolites. *Collect. Czech. Chem. Commun.* (in press).
19. Jiráťová K., Morávková L., Urbanová M., Pola J.: Laser induced oxidative coupling of methane. Effect of catalyst composition. *React. Kinet. Catal. Lett.* (in press).
20. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. *Catal. Lett.* (in press).
21. Jiráťová K., Kostova N. G., Sow B., Spojakina A. A.: Catalytic oxidation of ethanol in the presence of silica supported salts of phosphomolybdic acid. *Bulg. Chem. Commun.* (in press).
22. 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.* (in press).
23. Kostova N. G., Spojakina A. A., Jiráťová K.: Irradiation effect on HDS of Mo/Al₂O₃ catalysts. *Bulg. Chem. Commun.* (in press).
24. 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.* (in press).
25. Ponec R., Amat L., Carbó-Dorca R.: Molecular basis of quantitative structure-properties (QSPR) relations. A quantum similarity approach. *J. Comp. Aided Mol. Design* (in press).
26. Ponec R., Bochicchio R.: Nonlinear pair population analysis. The study of basis set dependence. *Int. J. Quant. Chem.* (in press).
27. Ponec R., Carbó-Dorca R.: Chemical bonds from the condition of minimal pair fluctuation. Correlated case. *Int. J. Quant. Chem.* (in press).
28. Ponec R., Duben A. J.: Electron pairing and chemical bonds. Bonding in hypervalent molecules from the analysis of the fermi holes. *J. Comput. Chem.* (in press).
29. 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).

Review papers

30. Jiráťová K., Jirka I.: Evropský kongres o katalýze Europa Cat-3. (Czech) European Congress on Catalysis EuropaCat-3. *Chem. Prům.* (in press).

Monographs

31. Zdražil M.: Effects of catalyst composition and pretreatment on the product distribution in hydrodesulfurization, hydrodenitrogenation, hydrogenation and hydrodechlorination. "Transition Metal Sulphides, Chemistry and Catalysis", NATO ASI Series (Weber T., Prins R., Rutger A. van Santen, Eds.), pp. 273-309, Kluwer Acad. Publ., Dordrecht (1998).

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32. Cinibulk J., Vít Z.: HDN of pyridine and HDS of thiophene over alumina supported Ir catalyst. 4th Pannonian International Symposium on Catalysis, Abstracts p. 9, Smolenice Castle, Slovakia, 11-14 June (1998).
33. Galík A., Galíková A.: Vliv difúze na měření kinetiky adsorpce na mikrováhách CAHN D-200. (Czech) The influence of diffusion on the measurement of kinetics of adsorption using microbalances Cahn D-200. 25. konferencia SSCHI, Zborník p. 107, Jasná, Slovakia, 25-29 May (1998).

34. Galík A., Galíková A., Klusáček K.: Gravimetric transient response study of adsorption and reaction of propylamines on alumina. 15th International Symposium on Chemical Reaction Engineering, pp. 366-367, Newport Beach, USA, 13-16 September (1998).
35. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Simulace kombinovaného transportu plynu s kinetikou adsorpce s porézním katalyzátorem. (Czech) The simulation of combined gas transport with adsorption kinetics in porous catalyst. 25. konferencia SSCHI, Zborník p. 144, Jasná, Slovakia, 25-29 May (1998).
36. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Modeling of gas permeation in porous catalysts. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 2, p. 144, Praha, 23-28 August (1998).
37. Hejtmánek V., Čapek P., Šolcová O., Schneider P.: Dynamic gas transport in porous bidispersed alumina. XXXth Symposium on Catalysis, Po23, Praha, 2-4 November (1998).
38. Jiráťová K.: Catalytic combustion of volatile organic compounds. 4th Pannonian International Symposium on Catalysis, abstract P27, Smolenice, Slovakia, 11-14 June (1998).
39. Jiráťová K.: Catalytic combustion of volatile organic compounds. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 1, p. 52, Praha, 23-28 August (1998).
40. Klicpera T., Zdražil M.: High surface area MoO₃/MgO catalyst, preparation by the new slurry impregnation method and activity in sulphided state in hydrodesulphurization of benzothiophene. XXXth Symposium on Catalysis, abstract Po2, Praha, 2-4 November (1998).
41. Ponc R., Bochicchio R., Lain L., Torre A.: Estudios de análisis de población en closo-boranos, X₂B₃H₃ (X=N, CH, P, SiH, BH-): determinación de enlaces multicéntricos. (Span) Studies of population analysis in closo-boranes (X=N, CH, P, SiH, Bh-) determination of multicenter bonds. XXIV. International Congress of Theoretical Chemists of Latin Expression, Puebla, Mexico, 20-25 September (1998).
42. Šolcová O., Šnajdaufová H., Hejtmánek V., Schneider P.: Vícesložková difuze v pórech; vliv experimentálního uspořádání. (Czech) Multicomponent diffusion in pores; the influence of experimental arrangement. 25. konferencia SSCHI, Zborník p. 110, Jasná, Slovakia, 25-29 May (1998).
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44. Šolcová O., Šnajdaufová H., Hejtmánek V., Schneider P.: Ternary gas diffusion in porous materials. XXXth Symposium on Catalysis, Po22, Praha, 2-4 November (1998).
45. Vít Z.: Stoichiometry of reaction between MoO₃ and OH groups of alumina. 4th Pannonian International Symposium on Catalysis, Abstracts p. 61, Smolenice Castle, Slovakia, 11-14 June (1998).
46. Vít Z.: Limitations of the estimation of molybdena coverage in MoO₃/alumina catalysts from the amount of OH groups. XXXth Symposium on Catalysis, PO21, Praha, 2-4 November (1998).
47. Zdražil M.: Preparation of molybdenum based catalysts of monolayer type by new solvent assisted spreading method. 4th Pannonian International Symposium on Catalysis, Book of Abstracts PL 5, Smolenice Castle, Slovak Republic, 11-14 June (1998).

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: P. Mitschka, V. Pěnkavová, J. Vrba, K. Wichterle
Technical staff: S. Nováková,
Part time: J. Vejražka, A. Zemek
PhD student: A. Elguzli

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

Applied research

- Resources recycling

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. 12, 31, 32]

Experimental verification of CFD models in agitated vessels

(V. Sobolík, joint project with Institute of Hydrodynamics ASCR and CTU, Faculty of Mechanical Engineering; supported by GA ASCR, grant No. A 2060604)

The estimation of adjustable constants and the applicability ranges of k - ϵ , RNG and RSM models of turbulent flow in agitated systems from local velocity distributions measured by using the Laser-Doppler anemometry and electrodiffusion diagnostics. [Ref. 51]

Suspension mechanism in apparatuses with rotating agitators

(V. Sobolík, joint project with CTU, Faculty of Mechanical Engineering; supported by GA CR, grant No. 101/96/0340)

The velocities close to the vessel bottom and velocity gradients at the bottom affect essentially the fluidization of solid particles. The distribution of the velocity gradients is measured with simple and segmented electrodiffusion probes. [Refs. 33, 51]

Electrochemical sensors for flow measurements

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

Electrodiffusion technique (three-segment probes, software and hardware) has been developed and applied in different flow situations (sudden expansion and contraction, Taylor-Couette flow, impinging jet). [Refs. 34, 35, 38, 39]

Wave evolution on a falling viscoelastic film

(J. Tihon, joint project with the Institute for Hydrodynamics of ASCR; supported by GA CR, grant No. 104/96/0569)

Linear stability theory was developed for the wavy film flow of viscous liquids along inclined plate. Experimental data on the wave characteristics of the viscoelastic films were obtained at low inclination angles of the plate. [Refs. 18, 36, 37]

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; supported by the GA CR, grant No. 104/97/1170)

Hydraulic characteristics of the ejector loop reactor (rate of gas entrainment, gas holdup, rate of energy dissipation) were determined in a wide viscosity range of the liquid medium. Experimental data, demonstrating viscosity effect on the performance of the ejector distributor, will be further used for characterisation of working conditions in mass transfer measurements. Studies of bubble coalescence in viscous aqueous media proved that coalescence in such media could be significantly modified by addition of surface active substances (aliphatic alcohols). [Refs. 9, 14, 22, 25, 47, 49]

Gas-liquid reactor design and selection for complex rheology fluids in the fine chemicals, bioprocessing and pharmaceutical industries

(J. Zahradník, joint project with UMIST Manchester, UK and the Institute of Chemical Engineering, Bulgarian Academy of Sciences Sofia, Bulgaria; supported by the Commission of the European Communities under COPERNICUS contract No. CIPA-CT94-0179 and by the Ministry of Education of the Czech Republic, grant No. OK 320 (1998)).

The network-of-zones model has been successfully modified for application to bubble column reactors. The model allows spatial 3-D visualisation of distribution of bubble bed voidage, k_{La} and dissolved oxygen concentration in the column. The selected version of the model was applied for detailed evaluation of the performance of an industrial bubble column fermentor for citric acid production. [Refs. 21, 22, 28, 42, 43, 48, 50]

International cooperations

University of Tokyo, Tokyo, Japan: Chaotic hydrodynamics of bubble columns

Hokkaido University, Sapporo, Japan: Processing of coal sorbents containing heavy metals

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

Technical University of Munich, Munich, FRG: Shear stresses on rotating bodies
CNRS UPR 15, Paris, France: Electrodiffusion diagnostics of flow
LEGI / IMG, Grenoble, France: Taylor-Couette instabilities
LEMTA, INPL, Vandoeuvre les Nancy, France: Ekman vortices
University of Poitiers, France: Electrochemical sensors for flow measurements
Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria: Gas-liquid reactors for complex rheology fluids

Visits abroad

J. Drahoš: NIRE, NIMC, Tsukuba, Japan; Royal Institute of Technology, Stockholm, Sweden; TU Delft, Delft, The Netherlands; Opole University, Opole, Poland; TU Wroclaw, Wroclaw, Poland
M. Růžicka: Aston University, Birmingham, UK
V. Sobolík: Univ.of Poitiers (3 months); Univ.of La Rochelle (2 months)
J. Tihon: CNRS UPR 15, Paris, France; Technion, Haifa, Israel; Tel-Aviv Univ., Tel-Aviv, Israel
O. Wein: Univ. of Calgary, Calgary, Canada (2 months)
J. Zahradník: Aston University, Birmingham, UK; University of Birmingham, Birmingham, UK; UMIST Manchester, UK

Visitors

C. Freitas, University of Minho, Braga, Portugal (4 months)
J.A. Teixeira, University of Minho, Braga, Portugal
R. Mann, UMIST Manchester, UK
B. Tribollet, CNRS, UPR 15, Paris, France
N.H. Thomas, Aston University, Birmingham, UK
S.D. Vlaev, Inst.of Chem.Eng., Bulgarian Acad.Sci., Sofia, Bulgaria
V. Tovchigrechko, ITMO Minsk, Byelorussia (12 months)
C. McGuckin, Univ.of Belfast, N.Ireland - IAESTE student

Teaching

J. Drahoš: PICT, course "Fluid Mechanics" and postgraduate courses "Applied Statistical Analysis and Data Processing" and "Multiphase Reactors"
J. Tihon: PICT, postgraduate course "Drops, bubbles and particles"
O. Wein: TU Brno, course "Principles of Rheology"
J. Zahradník: TU Brno, course "Bioengineering" and PICT, postgraduate course "Multiphase Reactors"

Publications

Papers

1. Lutz M., Denk V., Wichterle K., Sobolík V.: Electrodiffusional flow diagnostics in a centrifugal pump. *J. Appl. Electrochem.* 28, 337-342 (1998).
2. Punčochář M., Vrba J., Drahoš J.: Membership function for modelling of hierarchical processes. *SAMS* 31, 195-203 (1998).
3. Sobolík V., Tihon J., Wein O., Wichterle K.: Calibration of electrodiffusion friction probes using voltage-step transient. *J. Appl. Electrochem.* 28, 329-335 (1998).
4. Vrba J.: Decomposition of aggregated fuzzy sets - case studies. *SAMS* 33, 157-177 (1998).
5. Wein O.: Diffusion-layer theory for flows under apparent wall slip. *Collect. Czech. Chem. Commun.* 63, 132-140 (1998).
6. Wichterle K., Mitschka P.: Relative shear deformation of non-Newtonian liquids in impeller induced flow. *Collect. Czech. Chem. Commun.* 63(12), 2092-2102 (1998).
7. Wichterlová J., Wein O., Kaštánek F.: Particle migration in a Helle-Shaw cell with non-parallel walls. *Collect. Czech. Chem. Commun.* 63, 870-880 (1998).
8. Green K. D., Macek T., Zahradník J., Thomas N. H.: Growth parameters of transformed roots. *Biotechnol. Lett.* (in press).
9. Havelka P., Linek V., Sinkule J., Zahradník J., Fialová M.: Hydrodynamic and mass transfer characteristics of ejector loop reactors. *Chem. Eng. Sci.* (in press).
10. Kaštánek F., Zahradník J., Drahoš J., Maléterová Y.: Fate of polychlorinated biphenyls and chlorinated aliphatic hydrocarbons in soil and ground water under field condition. *Environ. Eng. Policy* (in press).
11. Punčochář M., Drahoš J.: Fractal geometry: A tool for fuzzy reasoning. *Int. J. General Systems* (in press).
12. Růžička M.: On bubbles rising in line. *Int. J. Multiphase Flow* (in press).
13. Sobolík V.: Electrochemical study of Taylor-Couette flow by limiting diffusion current method. *Collect. Czech. Chem. Commun.* (in press).
14. van Dierendonck L. L., Zahradník J., Linek V.: Loop Venturi reactor-a feasible alternative to stirred tank reactors. *Ind. Eng. Chem. Res.* (in press).
15. Vrba J.: Mass transfer models with fuzzy parameters. *Int. J. Syst. Anal. Model. Simul.* (in press).
16. Vrba J.: Recycle processes - costs analysis and optimization. *SAMS* (in press).
17. Vrba J.: Recycle processes - A note on the convergency of their sequential steady-state simulation. *SAMS* (in press).
18. Wein O., Wichterlová J., Sobolík V.: Viskozita vodných roztoků polyglykolu EMKAROX HV 45. (Czech) Viscosity of aqueous solutions of polyglycol EMKAROX HV 45. *Chem. Prům.* (in press).
19. Wichterlová J., Rod V.: Dynamic behaviour of the mixer-settler cascade. Extractive separation of the rare earths. *Chem. Eng. Sci.* (in press).
20. Yano T., Kikuchi R., Tsutsumi A., Yoshida K., Punčochář M., Drahoš J.: Nonlinear hydrodynamics of three-phase reactors. *Kagaku Kogaku Ronbunshu* (in press).
21. Zahradník J., Kuncová G., Fialová M.: The effect of surface active additives on bubble coalescence and gas holdup in viscous aerated batches. *Chem. Eng. Sci.* (in press).
22. Zahradník J., Fialová M., Linek V.: The effect of surface active additives on bubble coalescence in aqueous media. *Chem. Eng. Sci.* (in press).

Monographs

23. Martemianov S., Gbahoue L., Evdokimov Yu. K., Sobolík V.: Etude du transfert de matiere a l'interface solide/liquide par la methode electrochimique. (Fr) Study of mass trasfer at solid/liquid interface using an electrochemical method. Ecole Superieure D'Ingenieurs (ESIP) De Poitiers, pp. 25, France (1998).

DrSc. Thesis

24. Drahoš J.: Analýza a diagnostika hydrodynamického režimu dvoufázových chemických reaktorů. (Czech) Analysis and diagnostic of hydrodynamic regimes of two-phase chemical reactors. Doktorská disertace, PICT Praha (1998).

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25. Havelka P., Linek V., Sinkule J., Zahradník J., Fialová M.: Hydrodynamic and mass transfer characteristics of ejector loop reactors. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 2, p. 5, Praha, 23-28 August (1998).
26. Kaštánek F., Zahradník J., Drahoš K., Maléterová Y.: Fate of polychlorinated biphenyls and chlorinated aliphatic hydrocarbons in soil and groundwater under field conditions. NATO ARW Tools and Methods for Pollution Prevention, Praha, 12-14 October (1998).
27. Kuncová G., Burkhard J., Pazlarová J., Demnerová K., Drahoš J., Kotlíková J., Chomát M., Matějec V., Tříška J., Vrchotová N.: Fiber-optic detection of polychlorinated biphenyls in water and oil. Europt(r)ode IV, Book of Abstracts, pp. 85-86, Munster, Germany, 29 March-1 April (1998).
28. Mann R., Vlaev D., Lossev V., Vlaev S. D., Zahradník J., Seichter P.: Fundamentals of gas-liquid mixing in an industrial Thylosin reactor. 8th International Summer School of Chemical Engineering, Proc. p. 229, Bulgaria, 3-9 Juni (1998).
29. Punčochář M., Veselý V., Horáček J., Mastná A., Schwarz J., Koutský B., Malecha J., Skoblja S.: Emissions during combustion of charcoal. 13th International Congress of Chemical and Process Engineering CHISA'98, P5. 86, 137, Praha, 23-28 August (1998).
30. Punčochář M., Veselý V., Drahoš J., Tsutsumi A., Yoshida K.: Formation of persistent organic polutants during the fluidized bed combustion. 6th Asian Conference on Fluidized-Bed and Three-Phase Reactors, Cheju, Korea, 8-12 December (1998).
31. Růžička M., Drahoš J., Zahradník J.: Hydrodynamické interakce bublin při simultánním bublení ze dvou otvorů. (Czech) Hydrodynamic interactions of bubbles at simultaneous bubbling from two orifices. 25. konferencia SSCHI, Zborník p. 158, Jasná, Slovakia, 25-29 May (1998).
32. Růžička M., Drahoš J., Zahradník J.: Interference of pressure signals at multiple bubble formation. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 3, p. 69, Praha, 23-28 August (1998).
33. Sobolík V., Fořt I., Rieger F., Nermut M., Pospíšil R.: Electrochemical measurement of velocity gradients at the vessel bottom with axial high-speed impeller and radial baffles. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 7, p. 25, Praha, 23-28 August (1998).
34. Tihon J., Deslouis C.: Studium přístěnné turbulence elektrodifúzní metodou. (Czech) Near-wall turbulence studied by the electrodiffusion method. 25. konferencia SSCHI, Zborník p. 86, Jasná, Slovakia, 25-29 May (1998).
35. Tihon J., Deslouis C., Tribollet B.: Structure of the near-wall turbulence in a drag-reducing flow. 5th European Rheology Conference 1998, p. 163, Portorož, Slovenia, 6-11 September (1998).

36. Tihon J., Wein O.: Stability of the viscoelastic film flow down an inclined plane. 5th European Rheology Conference 1998, p. 165, Portorož, Slovenia, 6-11 September (1998).
37. Tihon J., Wein O.: The stability of a non-newtonian film flowing down an inclined plane. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 7, p. 14, Praha, 23-28 August (1998).
38. Tihon J., Legrand J., Legentilhomme P.: Electrodiffusional diagnostics of backward-facing step flows. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 5, p. 85, Praha, 23-28 August (1998).
39. Tihon J., Deslouis C., Tribollet B.: Turbulent drag reduction by high polymers additives studied by the electrodiffusional technique. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 5, p. 86, Praha, 23-28 August (1998).
40. Vejražka J., Sobolík V.: Velocity gradient near stagnation point of impinging jet. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 5, p. 30, Praha 23-28 August (1998).
41. Veselý V., Punčochář M., Drahoš J.: Vliv popílku na tvorbu persistentních látek při spalování. (Czech) The influence of fly ash on the formation of persistent compounds during combustion. 25. konferencia SSCHI, Zborník p. 164, Jasná, Slovakia, 25-29 May (1998).
42. Vlaev D., Mann R., Lossev V., Vlaev S. D., Zahradník J., Seichter P.: Fundamentals of gas-liquid mixing and mass transfer in a triple-impeller stirred industrial bioreactor. IChemE Research Event 1998, Book of Abstracts, p. 53, Newcastle, 7-8 April (1998).
43. Vlaev S. D., Mann R., Vlaev D., Lossev V., Zahradník J., Seichter P.: Fundamentals of gas-liquid mixing in an industrial stirred bioreactor for antibiotics in Razgrad. 8th International Summer School of Chemical Engineering, Proc. p. 201, Bulgaria, 3-9 Juni (1998).
44. Wein O., Zanzotto L.: Comparison of the generalized Maxwell and Stastna model for characterizing dynamic moduli of modified asphalts. 5th European Rheology Conference 1998, p. 317, Portorož, Slovenia, 6-11 September (1998).
45. Wein O.: Apparent wall slip in rotational viscometry. 5th European Rheology Conference 1998, pp. 505-506, Portorož, Slovenia, 6-11 September (1998).
46. Wein O.: Rheometry and transport processes in microdisperse liquids. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 7, p. 9, Praha, 23-28 August (1998).
47. Zahradník J., Fialová M., Linek V.: Vliv povrchově aktivních aditiv na koalescenci bublin ve vodných médiích. (Czech) The effect of surface-active additives on bubble coalescence in aqueous media. 25. konferencia SSCHI, Zborník p. 142, Jasná, Slovakia, 25-29 May (1998).
48. Zahradník J., Kuncová G., Fialová M.: The effect of aliphatic alcohols on gas holdup in viscous aerated batches. 8th International Summer School of Chemical Engineering, Proc. p. 239, Bulgaria, 3-9 Juni (1998).
49. Zahradník J., Fialová M., Linek V.: The effect of surface active additives on bubble coalescence in aqueous media. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 2, p. 96, Praha, 23-28 August (1998).
50. Zahradník J., Kuncová G., Fialová M.: The effect of surface active additives on bubble coalescence and gas holdup in viscous aerated batches. 15th International Symposium on Chemical Reaction Engineering, pp. 528-529, Newport Beach, USA, 13-16 September (1998).
51. Sobolík V., Fořt I., Rieger F., Ditl P.: Velocity gradient components at bottom and wall of mixing vessel. 2nd European Congress of Chemical Engineering, Montpellier, France (in press).

Department of Biotechnology and Environmental Processes

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Part time: Y. Maléterová
Technical staff: K. Auerová, Z. Soukup, A. Surová
PhD students: T. Brányik, J. Kotlíková, H. Richterová, J. Szilva

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
- Catalysis by organometallic complexes in aqueous systems
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals

Applied research

- Pilot-scale sorption and biodegradation of PCBs from ground water
- Chemical modification of low molecular weight polybutadienes

Research projects

Catalysts for hydrogenation of lipids in cell membranes

(J. Čermák, supported by GA ASCR, grant No. A4072610)

Novel alkoxy-silyl-substituted pentamethylcyclopentadienyl rhodium(I) complexes with oligomethylene spacers of different length between the Cp* ring and the alkoxy-silyl functionality were prepared. Polysiloxane-bound complexes prepared from them by a sol-gel process exhibited catalytic activity in hydrogenation of crotonic acid in aqueous medium, which was used as a model reaction for hydrogenation of lipids in cells. [Ref. 24]

Environmental biotechnology and environmental chemical engineering

(F. Kaštánek, joint project with PICT)

Localities with old contamination of soil and ground water by polychlorinated biphenyls (PCB) and chlorinated ethenes (CIU) exhibit different rates and mechanisms of biodegradation and both qualitatively and quantitatively different occurrence of aerobic and anaerobic microorganisms. Criteria for feasibility of spontaneous degradation of CIU and PCB in ground water and soil have been formulated:

- a) congener analysis was applied to evaluate the long time exposure of individual congeners of PCBs in the environment. In the course of approx. 20 years the low change in congener composition could probably be due to slow biodegradation of light congeners in the relatively good oxygenated superficial layers of soil
- b) enhanced reductive dehalogenation of PCBs was accomplished by the solid-state fermentation in reactors of 15 cubic meters of volume. Efficiency of biodegradation of individual congeners was evaluated and limits of the method for its practical use were determined
- c) different reaction rates of CIU degradation in ground water have been ascribed to the presence and/or activity of specific anaerobic bacteria in field condition. In the environment, free of such specific anaerobic bacteria, the conditions are suitable neither for spontaneous nor for enhanced biodegradation of chlorinated ethenes. [Refs. 7, 8]

Study of bioreactors with immobilized cells for hydrocarbon degradation in waste waters

(G. Kuncová, joint project with PICT, supported by GA CR, grant No. 104/96/0459)

Continuous degradation of phenol by cells immobilized into silica gel, polyurethane foam and ceramic foam was studied in packed-bed, fluidized-bed and trickle-bed reactor. The highest phenol degradation rates were measured in the packed-bed reactor filled with ceramic foam package. However, due to gradual colonisation of the ceramic package, the reactor showed rather slow degradation rates especially during the first 3-4 days of its operation. The sol-gel technique made possible the deposition of a cell-rich silica layer on the surface of the macroporous ceramic support and enhanced the degradation efficiency from the beginning of the continuous degradation. [Ref. 1]

Dehalogenation of polychlorinated biphenyls by Fenton's reagent

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

The research was focused on the experimental choice of solvents increasing the solubility of degraded polychloroaromates and biphenyls in aqueous phase. Catalysts of phase transfer were also used to improve hydroxylation of chlorous substituted aromates. The effect of pH of reaction solution has been observed.

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. 1, 4, 22, 23, 27]

Microwave activation of chemical reactions on solid catalysts and supports

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

Study of heterogeneous reactions taking place on the surface of solids revealed that localised superheating was responsible for the rate enhancements and no specific activation occurred. Temperature gradients resulted from localised superheating were successfully eliminated by efficient stirring of solid reaction mixture. Reactions were extended to the field of solid state chemistry. In addition to the main project a new activation method of photochemical reactions by microwave irradiation has been studied using electrodeless lamps and a new photoreactor for organic synthesis was developed. [Refs. 11, 13-15, 18, 26]

Catalysis by transition metal complexes with azine ligands

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

A series of novel azine diphosphine ligands with different alkyl and aryl substituents on phosphorus atoms was prepared with the aim of influencing the steric parameters of the donor site. Binuclear methallyl palladium(II) complexes and mononuclear cationic nickel(II) complexes of those ligands were synthesized and characterized by multinuclear NMR spectroscopy and FAB mass spectrometry, crystal structures of one of the ligand derivatives (dioxide) and one of the nickel complexes were determined by X-ray diffraction. [Refs. 6, 16, 17]

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.

International cooperations

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

Institute of Geotechnique, SA Sci., 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

H. Richterová: Université de Paris-Sud, Paris, France

M. Hájek: Universität Dortmund, Germany, Institute of Geotechnique, SA Sci., Košice, Slovakia

V. Čírkva: University of Madison, USA (8 months)

J. Čermák: Instituto Superior Técnico, Lisbon, Portugal

G. Kuncová: University of Muenster, FRG, University of Paris VI, France, ENSAIA, Nancy, France (5 months)

Visitors

A. Loupy, A. Petit: Université de Paris-Sud, Paris, France
I. Murová, I. Florek: Institute of Geotechnique, SA Sci., Košice, Slovakia
M. Radoiu: National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania (4 months)
M.F.N.N. Carvalho: Instituto Superior Técnico, Lisbon, Portugal
B. Schelle: Gerhard-Mercator-University GH, Duisburg, FRG

Teaching

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

Publications

Papers

1. Brányik T., Kuncová G., Páca J., Demnerová K.: Encapsulation of microbial cells into silica gel. *J. Sol-Gel Sci. Technol.* 13, 283-287 (1998).
2. Podlaha J., Císařová I., Kvíčalová M., Schraml J.: Self-assembly of 4-nitrobenzhydroxamic acid in the crystal. *Supramol. Chem.* (1998).
3. Schraml J., Kvíčalová M., Blechta V., Řeřicha R., Rozenski J., Herdewijn P.: ^{29}Si NMR spectra of trimethylsilyl and tert-butyl dimethylsilyl derivatives of purines and pyrimidines. *Magn. Reson. Chem.* 36, 55-63 (1998).
4. Szilva J., Kuncová G., Patzák M., Dostálek P.: The application of sol-gel technique for preparation of heavy metal biosorbent from yeast cells. *J. Sol-Gel Sci. Technol.* 13, 289-294 (1998).
5. Wichterlová J., Wein O., Kaštánek F.: Particle migration in a Helle-Shaw cell with non-parallel walls. *Collect. Czech. Chem. Commun.* 63, 870-880 (1998).
6. Carvalho M. F. N. N., Čermák Jan, Francisco F. A., Pombeiro A. J. L., Šabata S.: Study of the redox properties of some palladium and nickel complexes with azine diphosphine type ligands. *Portugaliae Electrochimica Acta* (in press).
7. Kaštánek F., Zahradník J., Drahoš J., Maléterová Y.: Fate of polychlorinated biphenyls and chlorinated aliphatic hydrocarbons in soil and ground water under field condition. *Environ. Eng. Policy* (in press).
8. 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).
9. Schraml J., Kvíčalová M., Soukupová L., Blechta V.: Structure of silylated benzhydroxamic acids. *J. Mag. Res. Chem* (in press).
10. Zahradník J., Kuncová G., Fialová M.: The effect of surface active additives on bubble coalescence and gas holdup in viscous aerated batches. *Chem. Eng. Sci.* (in press).

Monographs

11. Čermák Jan, Hájek M., Hetflejš J., Včelák J.: International Conference on Microwave Chemistry. Sborník z konference, 123 pp., Praha, 6-11 September (1998).
12. Kaštánek F.: Bioinženýrství. (Czech) Bioengineering. ACADEMIA, Praha (in press).

Conferences

13. Brožek V., Dufek V., Hájek M.: Reactive sintering of BN-SiC-metal composites in a microwave field. International Conference on Microwave Chemistry, Book of Abstracts, P22, Praha, 6-11 September (1998).
14. Brožek V., Dufek V., Hájek M.: Microwave enhanced reactive sintering of composites on BN-SiC base. 1998 Powder Metallurgy World Congress and Exhibition, Vol. 4, pp. 164-167, Granada, Spain, 18-22 October (1998).
15. Církva V., Hájek M.: Microwave photoreactor for organic synthesis. International Conference on Microwave Chemistry, Book of Abstracts, P45, Praha, 6-11 September (1998).
16. Čermák Jan, Blechta V., Šabata S., Vojtíšek P., Carvalho M. F. N. N.: The synthesis and versatile chemistry of some nickel and palladium complexes with bis(diphenylphosphino) pinacolone azine. XVIIIth International Conference on Organometallic Chemistry, Book of Abstracts, Part I, DO42, Munich, 16-21 August (1998).
17. Čermák Jan, Šabata S., Vojtíšek P., Carvalho M. F. N. N.: Zerovalent nickel and palladium complexes of bis (diphenylphosphino)pinacoloneazine-formation of a new Pd-C bond by electron transfer to a coordinated alkyne. 11th International Symposium on Homogeneous Catalysis, Book of Abstracts, P. 101, St Andrews, Scotland, UK, 12-17 July (1998).
18. Hájek M.: Application of microwaves to heterogeneous catalysis. Application of Microwaves in Material Sciences and Solid State Chemistry, Dortmund, BRD, 17-18 March (1998).
19. Kaštánek F., Zahradník J., Drahoš K., Maléterová Y.: Fate of polychlorinated biphenyls and chlorinated aliphatic hydrocarbons in soil and groundwater under field conditions. NATO ARW Tools and Methods for Pollution Prevention, Praha, 12-14 October (1998).
20. Kaštánek F., Demnerová K., Burkhard J., Pazlarová J.: Fate of PCBs and volatile chlorinated hydrocarbons in contaminated soils and ground water in field conditions. 2nd International Seminar Biosorption and Bioremediation, Prague, August (1998).
21. Kaštánek P., Kaplánek R., Kaštánek F., Hetflejš J.: Zneškodňování nebezpečných organických látek sorbovaných na tuhých nosičích. (Czech) Decontamination of hazardous organic compounds sorbed at solids. International Conference WASTE Prague, May (1998).
22. Kuncová G., Burkhard J., Pazlarová J., Demnerová K., Drahoš J., Kotlíková J., Chomát M., Matějec V., Tříška J., Vrchotová N.: Fiber-optic detection of polychlorinated biphenyls in water and oil. Europt(r)ode IV, Book of Abstracts, pp. 85-86, Munster, Germany, 29 March-1 April (1998).
23. Kuncová G., Poncelet D., Burkhard J., Pazlarová J., Elsniye D.: Alginate beads coated with silica layer prepared by sol-gel technique. Application of the optical detection of polychlorinated biphenyls. Workshop Bioencapsulation VII, Easton, Maryland, USA, 20-23 November, full text in press (1998).
24. Kvíčalová M., Čermák Jan: Pentamethylcyclopentadiene-functionalized polysiloxanes and their rhodium complexes as hydrogenation catalysts in an aqueous medium. 11th International Symposium on Homogeneous Catalysis, Book of Abstracts, P. 102, St Andrews, Scotland, UK, 12-17 July (1998).
25. Pekárek V., Smolík J., Tydlitát V., Výška J., Příbyl J., Kilian J., Beneš J., Grabic R., Lojkásek M.: Testování obsahu polychlorovaných dioxinů a dibenzofuranů ve výfukových plynech zážehových motorů. (Czech) Tests on polychlorinated dibenzodioxins and dibenzofurans in gasoline engine emissions. 3rd International Symposium MOTOR FUEL'98, Proceedings, Vyhne, Slovakia, 25-29 May (1998).

26. Richterová H., Hájek M.: Localized superheating effects in heterogeneous reactions. International Conference on Microwave Chemistry, Book of Abstracts, OR4, Praha, 6-11 September (1998).
27. Schelle B., Dress P., Franke H., Kuncová G., Pazlarová J., Demnerová K., Burkhard J.: Application of a liquid core waveguide for early detection of PCB's. 8th Vienna Opt(r)ode Workshop, Book of Abstracts, pp. 71-72, Praha, 7-8 October (1998).
28. Schraml J., Blechta V., Kvičalová M.: Trimethylsilyl and tert-butyldimethylsilyl groups in ^{29}Si NMR tagging. 14th European Experimental NMR Conference, p. 151, Bled, Slovenia, 10-15 May (1998).
29. Výška J., Příbyl J., Pekárek V., Stach J., Tydlitát V., Smolík J., Grabic R., Lojkásek M., Kilián J., Beneš J.: Oznaczenie trwałych zanieczyszczeń organicznych w gazach spalinowych silników zapłonowych. (Pol) Determination of persistent organic pollutants in exhaust gases on the Otto engine. III Międzynarodowe sympozjum Dioksyny-człowiek-srodowisko, p. 1, Kraków, 17-18 September (1998).
30. Zahradník J., Kuncová G., Fialová M.: The effect of aliphatic alcohols on gas holdup in viscous aerated batches. 8th International Summer School of Chemical Engineering, Proc. p. 239, Bulgaria, 3-9 Juni (1998).
31. Zahradník J., Kuncová G., Fialová M.: The effect of surface active additives on bubble coalescence and gas holdup in viscous aerated batches. 15th International Symposium on Chemical Reaction Engineering, pp. 528-529, Newport Beach, USA, 13-16 September (1998).

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Fields of research

- Gas-solid reactions
- Gas-solid reactors and operations
- Fluidized bed combustion
- Particulate emissions from combustion processes
- Laser induced chemistry
- Laser induced chemical vapour deposition (CVD) of novel materials
- Atmospheric chemistry: reactions of ozone with olefinic pollutants
- Synthesis of nanoparticles *via* aerosol processes
- Transfer processes in dispersed systems
- Nucleation phenomena

Applied research

- Know-how for the combustion of waste organic materials in fluidized bed [Ref. 34]

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 [Refs. 21, 23]. Simultaneously, the effect was explored of combustion regime on the formation of organic pollutants on fly ashes with the attention to the evolution of PCDD/F precursors [Ref. 55]. Further, the emission factor of charcoal for PCDD/F was found [Ref. 54]. In the laboratory research, the program of fly ash dechlorination was finished. The dechlorination of

hexachlorobenzene on fly ash from MWI in the temperature range 150-350 °C was investigated. A mechanism of dechlorination was suggested. [Ref. 33]

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 will be developed and incorporated into tractable models of the reactors for contacting coal-gas with solid sorbents. [Refs. 18-20]

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.

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. 36, 37, 60]

Detection and predicting of different states of fluidization

(V. Veselý, supported by GA ASCR, grant No. A4072601)

The project is an experimental as well as theoretical effort to explore the intricate hydrodynamic behaviour of larger beds of solid particles fluidized with a gas. Pressure fluctuations have been measured at different positions in a bed by means of sensitive pressure probes. The resultant time series have been analysed off-line by evaluating their auto-correlations, power spectral density functions and probability density. [Ref. 12]

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. 41-43, 62, 63]

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

(K. Svoboda, supported by the EC in the program INCO-Copernicus PL975102, 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, 39, 43, 61-63]

Studies of atmospheric chemistry and air pollution

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

Studies on reaction of ozone with alkenes at ppm level in nitrogen atmosphere and air have been carried out to identify the products at different temperatures. It was revealed that secondary ozonides are important products, and their laser-induced homogeneous decomposition yields products of rearrangement. [Ref. 17]

Deposition of Si₂O and Si₂O/H films from the gas phase

(J. Pola, supported by GA CR, grant No. 203/96/1217)

Laser induced chemical vapour deposition was revealed to be a very efficient way of preparation of novel materials containing silicon. Si₂O and Si₂O/H films from different organosilicon compounds (e.g., disiloxane) are materials with potential applications as semi-conductors.

Laser induced decomposition of hydridodisiloxanes

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

IR laser induced gas-phase and liquid-phase decomposition of various polyhydridodisiloxanes are examined to reveal that these compounds afford a blend of polysiloxanes as formed via extrusion of silanones and their subsequent insertion into initial disiloxanes. In the liquid phases, this reaction of 1,3-diphenyldisiloxane is photosensitized and exhibits a simpler course than the conventional hot-wall-induced reaction. [Refs. 14, 26]

Laser induced synthesis of novel polymers

(J. Pola, supported by Ministry of education, youth and sport, grant No. ME192)

IR and nitrogen laser irradiation of mixtures of organosilicon and common monomers results in chemical deposition of novel organosilicon polymers containing tetravalent and elemental silicon. The unique formation of the latter is believed to be enhanced by multiphoton absorption in polymeric agglomerates. [Refs. 3, 4, 8, 27]

The improvement of organic photochemical reaction control by using lasers

(J. Pola, supported by Ministry of education, youth and sport, grant No. ME191)

Excimer laser photolysis of dialkyltelluriums and tellurophene in n-hexane affords nanostructures Te and Te/C particles surface of which is oxidized in atmosphere and whose content depends on the structure of the organotellurium precursor. [Refs. 7, 25]

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

(J. Pola, supported by Ministry of education, youth and sport, grant No. ME225)

Examination of the use of single tailored organosilicon precursors for chemical vapour deposition of polycarbosilanes and silicon carbide is under way. It has been revealed that tert-butylsilane decomposition by IR laser radiation is dominated by elimination of isobutene and formation of Si/C/H coatings. [Refs. 28, 29]

Laser induced decomposition of hydridosiloxanes

(J. Pola, NATO collaborative research grant)

The research carried out jointly with University of Crete. Infrared multiphoton and UV photolysis of methylhydridodisiloxanes is examined with the aim of elucidating the mechanism of these reactions and characterizing solid products.

Experimental study of the homogeneous nucleation kinetics in supersaturated vapors

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

The aim of the project is the experimental study of homogeneous nucleation kinetics in supersaturated vapors using a static diffusion chamber. A new approach to the determination of the nucleation rate in dependence on temperature and supersaturation in the chamber is used. The chamber and technique have been tested by measuring the dependence of homogeneous nucleation rates on temperature and supersaturation simultaneously in our laboratory and partner laboratory in USA. [Ref. 15]

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. In 1998, homogeneous particles of alumina and mixed silica-alumina particles by decomposition of aluminium tri-*sec*-butoxide and tetraethylorthosilicate were prepared and characterised by SEM and EDAX analysis. [Refs. 49, 50]

International cooperations

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, FRG: Pressurized fluidized bed combustion

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

Instituto de Estructura de la Materia, CSIC Madrid, Spain: IR laser deposition of SiC

City University of New York, New York, USA: Laser-produced catalytically active films

Technical University, Graz, Austria: Laser chemistry of alkylsilanes

NIRE, Tsukuba, Japan: Resources Recycling in Eastern Europe

Centre of Molecular and Macromolecular Studies, Lodz, Poland: Laser generation of silicon containing transients

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

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

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

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

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

DMT Essen, FRG: Pressurized fluidized bed combustion

Visits abroad

J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (5 months)

K. Svoboda, National Taiwan University, Taipei, Taiwan

V. V. Levinskij, KRICT, Taejon, Korea (3 months)

M. Hartman: Lehigh University, Bethlehem, USA

Visitors

R. Hillamo: Finnish Meteorological Institute, Helsinki, Finland

S. Grinshpun: University of Cincinnati, USA
T. Chiba: Hokkaido University, Sapporo, Japan
A. Ouchi: Institute of Materials and Chemical Research, Tsukuba, Japan
K. Hassler: Technical University, Graz, Austria
S. Graschy: Technical University, Graz, Austria
D. Ziolkowski: Institute of Physical Chemistry, PAS, Warsaw, Poland
J. Michalski: Institute of Physical Chemistry, PAS, Warsaw, Poland

Publications

Papers

1. Dřínek V., Urbanová M., Bastl Z., Gregora I., Vorlíček V., Šubrt J., Pola J.: IR laser induced chemical vapour deposition of carbonaceous phases from 3-butyn-2-one. *Carbon* 36 (5-6), 521-524 (1998).
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11. Smolík J., Schwarz J., Kulmala M.: Experimental determination of ventilation coefficient for 1-hexanol drops in air. *Atmos. Res.* 46, 361-369 (1998).
12. Trnka O., Hartman M.: On the influence of fluctuating flow rate upon the performance and behaviour of isothermal reacting systems. *Collect. Czech. Chem. Commun.* 63, 881-898 (1998).

13. Urbanová M., Bastl Z., Plzák Z., Šubrt J., Gregora I., Vorlíček V., Pola J.: Laser photolysis of liquid benzene and hexafluorobenzene: graphitic and polymeric carbon formation at ambient temperature. *Carbon* 36, 517-520 (1998).
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16. Čermák Jiří, Svoboda K., Trnka O., Drobník P.: Tvorba a redukce NO a N₂O při fluidním spalování uhlí. (Czech) Formation and reduction of NO and N₂O from fluidized bed combustion of coal. *Ropa a uhlíe (Petroleum & Coal)* (in press).
17. Fajgar R., Vitek J., Haas Y., Pola J.: Definitive evidence of the formation of secondary ozonides in the ozonation of alkenes in the gas phase. *J. Chem. Soc., Perkin 2* (in press).
18. Hartman M., Trnka O., Svoboda K.: Potential of calcium oxide for removal of hydrogen sulphide and carbonyl sulphide from coal gas. *Fuel* (in press).
19. Hartman M., Trnka O., Svoboda K.: Essential factors in removing carbonyl sulphide from coal gas with lime and limestone. *Chem. Papers* (in press).
20. Hartman M., Svoboda K., Trnka O.: Effect of water vapour on the equilibrium between CaO and COS in coal gas. *Collect. Czech. Chem. Commun.* (in press).
21. 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).
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23. Kučera J., Havránek V., Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Šantroch J.: INAA and OIXE of atmospheric and combustion aerosols. *Biol. Trace Element Res.* (in press).
24. Levdanskij V. V., Moravec P., Smolík J.: Rost chastits pri khimicheskom osazhdenii iz gazovoi fazy. (Russ) Particle growth in chemical vapour deposition. *Inzh. Fyz. Zh. (J. Eng. Phys.)* (in press).
25. Ouchi A., Yamamoto K., Koga Y., Pola J.: Deposition of nanostructured Te and Te/C particles by laser photolysis of organotelluriums in the liquid phase. *J. Mater. Chem.* (in press).
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28. Pola J., Plzák Z., Ouchi A., Kupčík J., Koga Y.: CO₂ laser photosensitized decomposition of 1,3-diphenyldisiloxane in the liquid phase: formation of poly(phenylsiloxanes) via extrusion/insertion of phenylsilanone. *J. Organometal. Chem.* (in press).
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30. Punčochář M., Drahoš J.: Fractal geometry: A tool for fuzzy reasoning. *Int. J. General Systems* (in press).
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32. 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.* (in press).
33. Stach J., Pekárek V., Endršt R., Hetflejš J.: Dechlorination of hexachlorbenzene on MWI fly ash. *Chemosphere* (in press).
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41. Svoboda K., Hartman M., Čermák Jiří: Combustion processes-solid and liquid charring fuels. *Acta Montana, ser. B* (in press).

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42. Svoboda K., Kepák F.: Energetika a životní prostředí. (Czech) Production of energy and protection of environment. *Universita J. E. Purkyně, Fakulta P, Ústí nad Labem* (in press).

Conferences

43. Čermák Jiří, Svoboda K., Trnka O.: Jednoduchý model tvorby emisí oxidu dusnatého pro spalování kapalných paliv ve fluidní vrstvě za zvýšeného tlaku. (Czech) A simple model of formation of nitric oxide emissions in combustion of liquid fuels under elevated pressure. 25. konference SSCHI, Zborník p. 140, Jasná, Slovakia, 25-29 May (1998).
44. Havránek V., Kučera J., Voseček V., Horáková J., Smolík J., Schwarz J., Sýkorová I.: Matrix effects in PIXE analysis of aerosol and ash samples. *International Conference on Nuclear Analytical Methods in the Life Science (NAMLS)*, Beijing, China, 26-30 October (1998).
45. Khachatryan L., Pola J.: Comparative study of ArF laser-induced photolysis of disiloxanes in the gas phase. *15th International Symposium on Gas Kinetics, Book of Abstracts*, p. 199, Bilbao, Spain, 6-10 September (1998).
46. Kučera J., Havránek V., Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Šantroch J.: INAA and PIXE of combustion and atmospheric aerosols. *International Conference on*

- Nuclear Analytical Methods in the Life Science (NAMLS), Beijing, China, 23-30 October (1998).
47. Levdansky V. V., Moravec P., Smolík J., Ždímal V.: Particle growth in deposition from gas phase. IV International School-seminar Nonequilibrium processes and Their Application, Contributed papers pp. 26-28, Minsk, Belarus, 1-6 September (1998).
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 55. Punčochář M., Veselý V., Drahoš J., Tsutsumi A., Yoshida K.: Formation of persistent organic pollutants during the fluidized bed combustion. 6th Asian Conference on Fluidized-Bed and Three-Phase Reactors, Cheju, Korea, 8-12 December (1998).
 56. Schwarz J., Smolík J., Veselý V., Kugler J., Sýkorová I., Kučera J., Havránek V.: Reduction of toxic elements emissions from AFBC combustion of lignites. 13th International Congress of Chemical and Process Engineering CHISA'98, Summaries 1, p. 129, Praha, 23-28 August (1998).
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 60. Svoboda K., Čermák Jiří, Hartman M.: Emisní zdroje těžkých kovů v ČR a možnosti omezování jejich emisí. (Czech) Emissions of heavy metals in Czech Republic and possibilities of their reduction. 25. konferencia SSCHI, Zborník p. 51, Jasná, Slovakia, 25-29 May (1998).

61. Svoboda K., Hartman M., Čermák Jiří: Combustion mechanisms - solid phase: structural changes, heterogeneous reactions and emissions. NATO Adv. Study Inst., Maratea, Italy, 14-25 September (1998).
62. Svoboda K., Čermák Jiří, Veselý V.: NO_x chemistry and emissions. Heterogeneous reactions II. (N₂O). NATO Adv. Study Inst., Maratea, Italy, 14-25 September (1998).
63. Svoboda K., Čermák Jiří, Trnka O.: NO_x chemistry and emissions - solid fuels. Heterogeneous reactions I. (NO + NO₂). NATO Adv. Study Inst., Maratea, Italy, 14-25 September (1998).
64. Veselý V., Punčochář M., Drahoš J.: Vliv popílku na tvorbu persistentních látek při spalování. (Czech) The influence of fly ash on the formation of persistent compounds during combustion. 25. konferencia SSCHI, Zborník p. 164, Jasná, Slovakia, 25-29 May (1998).
65. Výška J., Příbyl J., Pekárek V., Stach J., Tydlitát V., Smolík J., Grabic R., Lojkásek M., Kilián J., Beneš J.: Oznaczenie trwałych zanieczyszczeń organicznych w gazach spalinowych silników zapłonowych. (Pl) Determination of persistent organic pollutants in exhaust gases of the Otto engine. III Miedzynarodowe sympozjum Dioksiny - czlowiek - srodowisko, p. 1, Kraków, 17-18 September (1998).

Department of Analytical Chemistry

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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. 203/96/0567)

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. 4, 7, 10]

Derivatives of Hydroxylamine, Solid State and Solution Structure

(J. Schraml, supported by GA ASCR, grant No. A4072605)

A study of extensive series of hydroxylamine derivatives by ^1H , ^{13}C , ^{29}Si and ^{15}N NMR spectroscopy in solution and by X-ray diffraction in the solid state. The aim of the project is to determine the factors responsible for the structure variation. [Refs. 8, 9, 11]

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.

International cooperations

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, Bulgarian Academy of Sciences, 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., Kalisz T., Sedláček J., Blechta V., Matějka P.: Polymerization of nitrophenyl propargyl ethers with transition metal catalysts and characterization of polymers. *Polymer* 39(18), 4443-4447 (1998).
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