

Academy of Sciences of the Czech Republic

**Institute of Chemical Process  
Fundamentals**

**Prague**

ANNUAL REPORT 1997

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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 16)
- Department of Multiphase Reactors (page 22)
- Department of Biotechnology and Environmental Processes (page 29)
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- Department of Analytical Chemistry (page 43)

## STAFF

(31 December 1997)

Category	Number of Employees
Research □	113 □
Technical □	21 □
Administrative □	20 □
Services □	20 □

## BUDGET 1997

(in thousands of Kč; 35 Kč = 1 US\$, approx.)

Institutional support from National Budget	42 807
Research funds from Grant Agencies	14 772
Contracts with industry	1 586
Total	59 165

### 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: S. Aleksovski, M. Chačaturjan, V. Staněk, H. Vychodilová  
Technical staff: A. Kadlecová, D. Karfik, 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 applicability of polymer adsorbents and catalyst carriers
- 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; solubilities of liquids in dense CO<sub>2</sub> with entrainer

### Applied research

- Extraction aided determination of organic pollutants in waters
- Extraction refining of phenols from tars
- Preparation of corundum support for ceramic membranes
- Evaluation of commercial ion exchanger catalysts for bisphenol A synthesis

### 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, and by GA CR, grant No. 104/96/0582)

Solvent impregnated resins prepared by supporting dialkyldithiophosphoric acid (DADTPA) on functionalized polymer carriers were investigated [Ref. 3]. 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 [Refs. 12, 13].

### **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. 14, 17]

### **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. [Ref. 7]

### **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 acid - 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. Conditions of the third phase formation in systems citric acid-amine salt - modifier - inert diluent were investigated, and a correlation for equilibrium systems (1,1)-acid-amine salt - modifier - inert diluent was developed. [Refs. 2, 4, 8]

### **Supercritical fluid extraction - experiment and modeling**

(H. Sovová, supported by ICPF ASCR)

Experimental data on high-pressure solubility of squalane, dinonyl phthalate and glycerol in carbon dioxide were published [Ref. 5], and effect of entrainers on the solubility was measured and correlated [Refs. 6, 18]. Experiments in supercritical fluid extraction of essential oils (peppermint, wild thyme, iris, sweet basil, tarragon) were focused on obtaining data for mathematical modeling of the process.

## **International cooperations**

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

Laboratoire de Chimie-Physique Macromoléculaire, ENSIC-CNRS, Nancy, France: Membrane separation

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

K. Jeřábek: Universities of Padua and L'Aquila, Italy; Bayer A.G., Leverkusen, FRG; Rohm and Haas Comp., Philadelphia, USA  
H. Sovová: Macedonian Academy of Sciences and Arts; University of Skopje, Macedonia  
P. Uchytíl: Hiroshima University, Japan (2 months); University of Swansea and University of Glasgow, Great Britain; Otto von Guericke University of Magdeburg, FRG; Tsing Hua University, Hsinchu, Taiwan; Korea Research Institute of Chemical Technology, Taejon, South Korea

## Visitors

A. D'Archivio, L. Galantini, University of L'Aquila, Italy  
R. Kita, University of Tennessee, USA (2 months)  
A. Strikovskiy, Weizmann Institute of Science, Rehovot, Israel  
I. Mishonov, Institute of Chemical Engineering, Sofia, Bulgaria.  
R. Soria, SCT, Tarbes, France

## Teaching

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

## Publications

### Papers

1. Jeřábek K., Prokop Z., Revillon A.: Adsorption-assisted catalysts. *React. Func. Polym.* 33, 103-108 (1997).
2. Procházka J., Heyberger A., Volaufová E.: Amine extraction of hydroxycarboxylic acids. 3. Effect of modifiers on citric acid extraction. *Ind. Eng. Chem. Res.* 36, 2799-2807 (1997).

3. Strikovský A. G., Jeřábek K., Cortina J. L., Warshawsky A.: Solvent impregnated resins via acid-base interaction of poly(4-vinylpyridine) resin and di(2-ethylhexyl)-dithiophosphoric acid. *Solv. Extr. Ion Exch.* 15, 259-283 (1997).
4. Heyberger A., Procházka J., Volaufová E.: Extraction of citric acid with tertiary amine - third phase formation. *Chem. Eng. Sci.* 53, 515-521(1997).
5. Sovová H., Jež J., Chačaturjan M.: Solubility of squalane, dinonyl phthalate and glycerol in supercritical CO<sub>2</sub>. *Fluid Phase Equilib.* 137, 185-191 (1997).
6. Sovová H., Komers R., Rat V., Chačaturjan M., Vlček D.: Solubility of squalane and dinonyl phthalate in CO<sub>2</sub> with entrainers. *J. Supercrit. Fluids* (in press).
7. Staněk V., Jiříčný V.: Experimental observation of pressure drop overshoot following an onset of gas flow in counter-current beds. *Chem. Eng. J.* (in press).
8. Tomovská R., Popovská F., Volaufová E., Heyberger A., Procházka J.: Extraction of tartaric acid with trialkylamine. *Collect. Czech. Chem. Commun.* (in press).
9. Tuchlenski A., Uchytíl P., Seidel-Morgenstern A.: An experimental study of combined gas phase and surface diffusion in porous glass. *J. Membr. Sci.* (in press).

#### Review papers

10. Corain B., Zecca M., Jeřábek K.: Catalysis and polymer networks. *Chem. Rev.* (in press).

#### Patents

11. Jeřábek K., Prokop Z.: Způsob výroby bisfenolů. (Czech) Method for production of bisphenols. *Czech. Pat. Appl.* 330-97 (1997).
12. Jeřábek K., Warshawsky A., Strikovský A.: Selektivní sorbent pro separaci iontů těžkých kovů a způsob jeho přípravy. (Czech) Selective sorbent for separation of heavy metal ions and method for its preparation. *Czech. Pat. Appl.* 3012-97 (1997).
13. Warshawsky A., Strikovský A., Jeřábek K.: Selective sorbent for separation of heavy metal ions and method for its preparation. *Israel Pat. Appl.* 121369 (1997).

#### Conferences

14. Corain B., D'Archivio A., Galantini L., Jeřábek K., Králík M., Lora S., Palma G., Zecca M.: Metal catalysis inside microporous synthetic resins: some recent results. *Supported Reagents and Catalysts in Chemistry*, Limerick, Ireland, 8-11 July (1997).
15. Jeřábek K.: Relations between adsorbent morphology and mechanism of adsorption in solid-liquid systems. *NATO ASI Series 491 "Physical adsorption: Experiment, theory and application"*, pp. 587-590, Dordrecht, FRG (1997).
16. Jeřábek K.: Polymer carriers viewed as microreactors. *Gordon Conference on Reactive Polymers, Ion Exchangers and Adsorbents*, Henniker, USA, 20-25 July (1997).
17. Králík M., Fišera R., Hronec M., Jeřábek K., Zecca M., Corain B.: Modelling of deactivation of supported palladium catalysts in the hydrogenation of aromatic nitrocompounds. *Third European Congress on Catalysis EuropaCat-3*, Abstr., Vol. 2, p. 768, Kraków, Poland, 31 August-6 September (1997).
18. Sovová H., Rat V., Chačaturjan M., Vlček D.: Solubility of squalane, dinonyl phthalate and glycerol in CO<sub>2</sub> with entrainers. *4th Italian Conference on Supercritical Fluids and Their Applications*, pp. 403-408, Capri, Italy, 7-10 September (1997).
19. Volaufová E., Heyberger A., Procházka J.: Aminová extrakce kyseliny citronové a mléčné. (Czech) Amine extraction of citric and lactic acids. *24. konferencia SSCHI*, Zborník p. 139, Častá-Papiernička, Slovakia, 15-19 June (1997).



## E. Hála Laboratory of Thermodynamics

Head: I. Wichterle  
Deputy: K. Aim  
Research staff: O. Drábek, J. Kolafa, J. Linek, M. Lísal, I. Nezbeda, J. Pavlíček, J. Slovák,  
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

### Fields of research

- Determination of fluid phase equilibrium data at low, normal, and high pressures
- 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
- Determination of pressure dependence of boiling temperatures of aqueous solutions of N-methylmorpholine N-oxide

### 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)

Thermodynamic and structural data for model liquids of particles interacting via the EXP-6 potential and of homo- and hetero-nuclear square-well diatomics have been generated by molecular simulations. For the EXP-6 fluid, predictive power of the Weeks-Chandler-Andersen and optimized reference hyper-netted chain theories has been assessed and the fluid-solid boundary localized. Applicability of the two-centre dipolar Lennard-Jones model fluid to represent thermodynamic properties along the vapour-liquid coexistence region of short-chain halogenated hydrocarbons has been investigated. [Refs. 9, 16, 18, 21-24, 39, 40]

**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 diethyl phthalate, 1-pentanol, 1-heptanol, 1-tetradecanol and ethylbenzene have been measured by high precision comparative ebulliometry over the approximate pressure range of 5 to 100 kPa. A simple static technique was used to determine the vapour pressures of aqueous solutions of N-methylmorpholine N-oxide. [Refs. 15, 28, 37, 43]

### **Equilibrium behaviour of fluids constituted of anisotropic molecules**

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

Vapour-liquid equilibrium and excess volume data have been measured for a series of systems of the type chlorinated hydrocarbon plus non-polar component. Full second-order perturbation theory for fluids constituted of anisotropic molecules has been extended in a consistent way to mixtures and successfully examined for its ability 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. [Refs. 3, 26, 32, 36, 42]

### **Pressure-volume-temperature behaviour of liquids and liquid mixtures**

(J. Linek, supported by ICPF ASCR)

Densities of liquids and excess volumes of liquid mixtures 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. 3, 33, 38]

### **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 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. 11, 14, 31, 34]

### **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. 10-14, 19, 21, 34]

### **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. [Refs. 10, 12, 13, 16, 21]

### **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 binary systems (naphthene + alkyl alkanoate, ketone + chloroalkane, chloroketone + hydrocarbon) have been carried out. Data processing: New group (disperse and quasichemical) contributions were evaluated for the DISQUAC prediction methods. Data base: Vapour-liquid

equilibrium data bibliography was supplemented by the end of 1996. [Refs. 1-4, 32, 33, 38, 44, 45]

## International cooperations

DICAMP, University of Trieste, Trieste, Italy: Phase equilibria for supercritical fluid technology  
University of Guelph, Guelph, Canada: Statistical mechanics of fluids  
Universität Erlangen, Erlangen, FRG: Equation of state and chemical equilibrium  
Sonderforschungsbereich, Universität Leipzig, Leipzig, FRG: Simulation of phase and reaction equilibria in inhomogeneous fluids (joint project).  
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  
Northwestern University, Evanston, Illinois, USA: Molecular dynamics studies of proteins  
University of Oklahoma, Norman, Oklahoma, USA: Molecular theories of solutions of electrolytes

## Visits abroad

K. Aim: Universidad Autónoma Metropolitana, Universidad Nacional Autónoma de Mexico, Instituto Mexicano del Petroleo, CINVESTAV, Mexico City; Universidad de Guanajuato, León, Mexico; University of Surrey, Guildford, UK; University of California, Berkeley, USA  
J. Kolafa: University of Odense, Odense, Denmark (1 month)  
M. Lísal: University of California, Berkeley, USA; Cornell University, Ithaca, USA  
I. Nezbeda: University of Guelph, Guelph, Canada; University of Oklahoma, Norman, USA; University of Sheffield, Sheffield, UK; University of Bangor, Bangor, UK; Agriculture University, Vienna, Austria  
J. Pavlíček: Universität Erlangen, Erlangen, FRG (12 months)  
I. Wichterle: Babes-Bolyai University, Cluj, Romania

## Visitors

A. Dahmani: Université de Science et Technologie, Alger, Algeria (2 months)  
L. L. Lee: University of Oklahoma, Norman, Oklahoma, USA  
M. Teodorescu: Romanian Academy of Sciences, Bucharest, Romania (8 months)  
H. Vörtler: Universität Leipzig, Leipzig, FRG

## Teaching

- K. Aim: PICT, postgraduate courses "Applied statistical analysis and data processing", "Applied statistical thermodynamics of fluid systems", "Experimental methods for determination of phase equilibria"
- T. Boublík: CU, courses "Basic physical chemistry", "Advanced chemical thermodynamics", and "Statistical thermodynamics"
- I. Nezbeda: Purkyně University, courses: "Analytical mechanics", "Introduction to computer simulations"
- I. Nezbeda: CU, course: "Computer simulations"

## Publications

### Papers

1. Dahmani O., Wichterle I., Ait-Kaci A.: Isothermal vapour-liquid equilibria for binary systems of C4 alkyl chlorides with n-heptane, toluene and methylcyclohexane at 323.15 and 333.15 K. *Fluid Phase Equilib.* 124, 135-146 (1996); Erratum: 131, 311 (1997).
2. Dahmani O., Wichterle I., Ait-Kaci A.: DISQUAC and UNIFAC group interaction parameters for chloroalkanes. *Fluid Phase Equilib.* 132, 15-20 (1997).
3. Dahmani O., Linek J.: Excess volumes of some binary mixtures containing 1-chlorobutane, 2-chlorobutane, 2-chloro-2-methylpropane, heptane, toluene or methylcyclohexane at 298.15 K. *ELDATA: Int. Electron. J. Phys.-Chem. Data* 2, 175-184 (1996), published (1997).
4. Dahmani O., Wichterle I., Ait-Kaci A.: Isothermal vapour-liquid equilibria for ternary and quaternary systems of butyl chlorides with n-heptane, toluene and methylcyclohexane at 323.15 K. *Fluid Phase Equilib.* 138, 213-230 (1997).
5. Kotrla M., Předota M.: Interplay between kinetic roughening and phase ordering. *Europhys. Letters* 39, 251-256 (1997).
6. Lísál M., Vacek V.: Effective potentials for liquid simulation of the alternative refrigerants HFC-134a (CF<sub>3</sub>CH<sub>2</sub>F) and HFC-125 (CF<sub>3</sub>CHF<sub>2</sub>). *Fluid Phase Equilib.* 127, 83-102 (1997).
7. Lísál M., Budinský R., Vacek V.: Vapour-liquid equilibria for dipolar two-centre Lennard-Jones fluids by Gibbs-Duhem integration. *Fluid Phase Equilib.* 135, 193-207 (1997).
8. Lísál M., Vacek V.: Direct evaluation of solid-liquid equilibria by molecular dynamics using Gibbs-Duhem integration. *Molec. Simulations* 19, 43-61 (1997).
9. Lísál M., Vacek V., Černý F.: Molecular dynamics simulation study on freezing of two-centre Lennard-Jones model of diatomic fluids. *Acta Polytech.* (in press).
10. Nezbeda I., Kolafa J., Smith W.R.: Molecular theory of phase equilibria in model and real associated mixtures. III. Binary solutions of inert gases and n-alkanes in ammonia and methanol. *Fluid Phase Equilib.* 130, 133-156 (1997).
11. Nezbeda I., Slovák J.: A family of primitive models of water: Three-, four-, and five-site models. *Molec. Phys.* 90, 353-372 (1997).
12. Nezbeda I.: Fluids of pseudo-hard bodies. *Molec. Phys.* 90, 661-664 (1997).
13. Nezbeda I., Kolafa J., Smith W.R.: Global phase diagrams of binary mixtures. Systematic basis for describing types of phase equilibrium phenomena. *J. Chem. Soc., Faraday Trans.* 93(17), 3073-3080 (1997).
14. Slovák J., Nezbeda I.: Extended five-site primitive models of water: theory and computer simulations. *Molec. Phys.* 91, 1125-1135 (1997).

15. Strnad M., Martins-Costa M.T.C., Millot C., Tunon I., Ruiz-Lopez M.F., Rivail J.L.: Molecular dynamics simulations of elementary chemical processes in liquid water using combined density functional and molecular mechanics potentials. II. Charge separation processes. *J. Chem. Phys.* 106, 3643-3657 (1997).
16. Vörtler H.L., Nezbeda I., Lísal M.: The Exp-6 potential fluid at very high pressures. Computer simulations and theory. *Molec. Phys.* 92, 813-824 (1997).
17. Aim K.: Vapor pressures of 2-chlorotoluene and 4-chlorotoluene and relative volatility in their binary system. *Thermochim. Acta* (in press).
18. Aim K.: On practical equations of state for methanol based on molecular theory. *Fluid Phase Equilib.* (in press).
19. 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.* (in press).
20. Kotrla M., Předota M., Slanina F.: Kinetic roughening and phase ordering in the two-components growth model. *Surface Sci.* (in press).
21. Lísal M., Nezbeda I., Vörtler H.L.: Fluid-solid boundary of the compressed EXP-6 fluids. *Fluid Phase Equilib.* (in press).
22. Lísal M., Nezbeda I.: Pure fluids of homo-and hetero-nuclear square-well diatomics. I. Computer simulation study. *Molec. Phys.* (in press).
23. Lísal M., Budinský R., Vacek V., Aim K.: Vapour-liquid equilibria of alternative refrigerants from dipolar two-centre Lennard-Jones fluids. *Int. J. Thermophys.* (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.: Towards a first-principle theory of water. *Chem. Phys. Lett.* (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., Kalyuzhnyi Yu.V.: Fluid of pseudo hard bodies. II. Reference models for water, methanol and ammonia. *Molec. Phys.* (in press).
28. 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* (in press).
29. Smith W.R., Nezbeda I., Strnad M., Tříška B.: The reaction ensemble method for the computer simulation of chemical and phase equilibria. II. Diatomic formation reactions and chemical potentials of ternary fused-hard-sphere systems. *J. Chem. Phys.* (in press).
30. Strnad M., Nezbeda I.: Extended Gibbs ensemble: a set of Gibbs ensembles with a fluctuating particle. *Molec. Simulations* (in press).
31. Strnad M., Nezbeda I.: Extended primitive models of water revisited. *Molec. Phys.* (in press).
32. 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-tetrachloroethane binary mixtures. *Fluid Phase Equilib.* (in press).
33. 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 at 298.15 K. *Fluid Phase Equilib.* (in press).

#### Review papers

34. Nezbeda I.: Simple short-ranged models of water and their application. A review. *J. Molec. Liquids* 73, 74, 317-336 (1997).

#### Monographs

35. Aim K., Cortesi A., Fermeglia M.: Solids and liquids in supercritical fluids. In: The experimental determination of solubilities (J.-J. Counioux, G.T. Hefter and C.L. Young, Eds.), Butterworth (in press).

#### Conferences

36. Aim K., Lísal M., Pavlíček J.: Thermodynamic properties of some halogenated ethane derivatives from the statistical-thermodynamic theory using simple interaction potentials. 16th European Seminar on Applied Thermodynamics, pp. 92-93, Pont-a-Mousson, France, 19-22 June (1997).
37. Aim K.: Applicability of the statistical thermodynamic theory to the modelling of the behaviour of real fluid systems. Abstr. Calorimetry, Exp. Thermodyn. Therm. Anal. Conf. CETTA 97, p. 20, Zakopane, Poland, 8-13 September (1997).
38. Linek J.: Densimetrické stanovení dodatkových objemů izomerních chlorbutanů s uhlovodíky. (Czech) Densimetric determination of excess volumes in isomeric chlorobutanes + hydrocarbon systems. 24. konferencia SSCHI, Zborník pp. 51-54, Častá-Papiernička, Slovakia, 15-19 June (1997).
39. Lísal M., Budinský R., Aim K.: Vapour-liquid equilibria of alternative refrigerants modelled as dipolar two-center Lennard-Jones fluids. 15th Experimental Thermodyn. Conf., p. 28, Guildford, UK, 16-18 April (1997).
40. Lísal M., Vacek V., Budinský R.: Vapour-liquid equilibria of alternative refrigerants by molecular dynamics. 13th Symposium on Thermophysical Properties, p. 406, Boulder, Colorado, USA, 22-27 June (1997).
41. Nezbeda I.: Properties of aqueous solutions of non-electrolytes from a molecular-based equation of state. 13th Symposium on Thermophysical Properties, Boulder, Colorado, USA, 22-27 June (1997).
42. Pavlíček J., Boublík T., Aim K.: Thermodynamics of alkanes modelled as Kihara fluids. 15th Experimental Thermodyn. Conf., p. 54, Guildford, UK, 16-18 April (1997).
43. Roháč V., Růžička V., Jose J., Aim K., Růžička K., Záborský M.: Thermodynamics properties of phthalate esters along vapor-liquid saturation curve. Abstr. Calorimetry, Exp. Thermodyn. Therm. Anal. Conf. CETTA 97, p. 206, Zakopane, Poland, 8-13 September (1997).
44. Wagner Z.: Moderní metody stanovení interakčních parametrů stavových rovnic z experimentálních dat rovnováhy kapalina-pára. (Czech) Modern methods of determination of EOS interaction parameters from experimental vapour-liquid equilibrium data. 24. konferencia SSCHI, Zborník pp. 55-58, Častá-Papiernička, Slovakia, 15-19 June (1997).
45. Wichterle I.: Generalization of EOS parameters for description of VLE at high pressures. Internat. Symp. Phase Equil., Cluj-Napoca, Romania, 2-3 June (1997).

## Department of Catalysis and Reaction Engineering

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

### Fields of research

- Catalytic combustion of volatile organic compounds in waste gases
- Transport processes in porous solids
- Hydrodechlorination over sulphides
- 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 process can be followed. The response signals from the automated cell are fed to a PC for numerical processing.

#### Graham cell for multicomponent gas diffusion in porous solids

(P. Schneider, supported by ICPF ASCR)

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.

### **Experimental verification of dynamic models of catalytic and separation processes**

(K. Klusáček, supported by ICPF ASCR)

The mechanism of adsorption and reaction of propylamines on  $\gamma$ -alumina was investigated using the gravimetric transient response method. The mechanism of adsorption accompanied by reaction was proposed, and optimised kinetic parameters were estimated. The experimental results were compared with the simulated system behaviour. [Ref. 32]

### **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/Al<sub>2</sub>O<sub>3</sub> sulphide catalysts prepared from various Ir salts was tested in parallel hydrodenitrogenation of pyridine and hydrodesulphurization of thiophene, and the dispersion of Ir was evaluated by chemisorption of hydrogen. The Ir sulphide catalysts were more active than the conventional NiMo/Al<sub>2</sub>O<sub>3</sub> sulphide system. The study was connected with the modification of the conventional NiMo sulphide system by addition of Ir. [Refs. 28, 42]

Active carbon supported transition metal sulphides across Periodic Table were tested in parallel hydrodechlorination of dichlorobenzene and hydrodesulphurization of methylthiophene. Activity and selectivity was discussed in relation to the disposal of chlorinated wastes and to the theory of catalysis over sulphides. [Refs. 2, 23, 31]

The MoO<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub> catalysts with variable loading were prepared by a new clean and simple method of impregnation with molybdic acid. No other chemicals besides MoO<sub>3</sub> and water were used in the impregnation. The catalysts were characterised by XRD, XPS, electron probe microanalysis, BET surface area and activity measurements in the hydrodesulphurization of thiophene. [Ref. 3]

### **Study of interaction between MoO<sub>3</sub> and OH groups of alumina**

(Z. Vít, supported by ICPF ASCR)

Deposition of MoO<sub>3</sub> on alumina is accompanied by the consumption of surface 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. The stoichiometry ratio OH/Mo decreased from 2 for the lowest loading to 0.8 at saturated loading of about 15% MoO<sub>3</sub>. This approach gives a valuable information about surface chemistry of the preparation of MoO<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub> catalysts. [Refs. 8, 41]

### **Oxosynthesis over NiMo sulphide catalysts**

(Z. Vít, supported by Region Rhone-Alpes, France)

Formation of ketones from ethylene, CO and H<sub>2</sub> over NiMo sulphide catalysts supported on alumina, MgO, ZrO<sub>2</sub> and active carbon was studied at 240-290 °C and 10 bar of pressure. The oxo selectivity was influenced by support, reaction temperature and H<sub>2</sub>S concentration in the feed. A selectivity of about 25% into diethylketone was achieved with a feed containing 0.4% H<sub>2</sub>S at 240 °C. [Ref. 7]



**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, and special attention was paid to the formation of the reaction intermediates (e.g., acetaldehyde). [Ref. 14]

**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. 5, 19]

**Chemical application of similarity indices**

(R. Ponec, supported by GA CR, grant No. 203/95/0650)

The project deals with the methodological development of quantitative similarity measures and their application for the rationalisation of structure-(re)activity relationships. [Refs. 16, 18, 20]

**Handbook of heterogeneous catalysis**

(M. Kraus, supported by GA CR, grant No. 203/95/0650)

The literature on substituent effects in heterogeneous catalysis, dehydrogenation of alcohols and elimination and addition reactions was summarised and discussed. [Refs. 25-27]

**International cooperations**

Theory of chemical reactivity: University of Liverpool, Liverpool, UK; Universität Hannover, Hannover, FRG; University of Buenos Aires, Buenos Aires, Argentina; Institute of Computation Chemistry, University of Girona, Spain

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

**Visits abroad**

K. JirátoVá: Indian Institute of Petroleum, Dehradun, India (2 weeks)

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

**Visitors**

R. Bochicchio, University of Buenos Aires, Buenos Aires, Argentina

A. Spojakina, Institute of Catalysis, Sofia, Bulgaria

D. Razus, Institute of Physical Chemistry, Bucharest, Romania

**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. Čapek P., Hejtmánek V., Šolcová O., Klusáček K., Schneider P.: Dynamics of gas transport in porous media. *Catal. Today* 38, 31-38 (1997).
2. Frimmel J., Zdražil M.: Comparative study of activity and selectivity of transition metal sulfides in parallel hydrodechlorination of dichlorobenzene and hydrodesulfurization of methylthiophene. *J. Catal.* 167, 286-295 (1997).
3. Hillerová E., Morishige H., Inamura K., Zdražil M.: Formation of monolayer of molybdena over alumina by unconventional slurry impregnation or solvent assisted spreading method. *Appl. Catal. A: General* 156, 1-17 (1997).
4. Jirátová K., Morávková L., Malecha J., Koutský B.: Ceramic foam-supported perovskites as catalysts for combustion of methane. *Collect. Czech. Chem. Commun.* 62, 875-883 (1997).
5. Ponec R.: Electron reorganization in chemical reactions. Bond order conservation vs multicenter bonding in the course of chemical reactions. *Collect. Czech. Chem. Commun.* 62, 1821-1831 (1997).
6. Šolcová O., Hejtmánek V., Schneider P.: Determination of effective diffusivities and transport parameters of porous solids in the single-pellet-string-column. *Catal. Today* 38, 71-77 (1997).
7. Vít Z., Portefaix J. L., Breyse M.: Transformation of ethene into ketones by CO and H<sub>2</sub> over NiMo sulfide catalysts. *Collect. Czech. Chem. Commun.* 62, 1015 (1997).
8. Vít Z., Zdražil M.: Stoichiometry of reaction between MoO<sub>3</sub> and OH groups of alumina. *J. Catal.* 171, 305 (1997).
9. 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).
10. 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).
11. Jirátová K., Morávková L., Urbanová M., Vitek J., Pola J.: Laser induced oxidative coupling of methane. *Catal. Lett.* (in press).
12. Jirátová K., Morávková L., Malecha J., Koutský B.: Perovskites on ceramic foams as catalysts for combustion of methane. *Collect. Czech. Chem. Commun.* (in press).
13. Jirátová K., Morávková L., Urbanová M., Vitek J., Pola J.: Laser induced oxidative coupling of methane. Effect of catalyst composition. *React. Kinet. Catal. Lett.* (in press).
14. Jirátová 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).
15. Kostova N. G., Spojakina A. A., Jirátová K.: Irradiation effect on HDS of Mo/Al<sub>2</sub>O<sub>3</sub> catalysts. *Bulg. Chem. Commun.* (in press).

16. Ponec R., Uhlík F.: Electron pairing and chemical bonds. On the accuracy of electron pair model of chemical bond. *J. Mol. Struct. (Theochem)* (in press).
17. Ponec R., Uhlík F., Cooper D. L., Jug K.: On the definitions of bond index and valence for correlated wave functions. *Croat. Chem. Acta* (in press).
18. Ponec R., Yuzhakov G., Haas Y., Samuni U.: Theoretical analysis of the stereoselectivity in the ozonolysis of olefins. Evidence for a modified Criegee intermediate. *J. Org. Chem.* (in press).
19. Ponec R., Mayer I.: Investigation of some properties of multicenter bond indices. *J. Phys. Chem.* (in press).
20. Ponec R.: Electron pairing and chemical bonds. Chemical structure, valences and structural similarities from the analysis of the Fermi hole. *J. Mat. Chem.* (in press).
21. Schneider P.: Effectiveness factor for nonisothermal catalytic reaction with combined transport processes: Maxwell-Stefan approach. *Collect. Czech. Chem. Commun.* (in press).
22. Zamlyny V., Kubelková L., Babůrek E., Jiráťová K., Nováková J.: Amination of cyclohexanol over metallosilicate based material. *Appl. Catal.* (in press).

#### Review papers

23. Frimmel J.: Katalytická hydrogenolýza chlorovaných látek na sulfidických katalyzátorech. (Czech) Catalytic hydrogenolysis of chlorinated compounds over sulphides. *Chem. Listy* 91, 840-845 (1997).

#### Monographs

24. Zdražil M.: Effects of catalyst composition and pretreatment on the product distribution in hydrodesulfurization, hydrodenitrogenation, hydrogenation and hydrodechlorination. *Challenges For Sulfides in Material Sciences and Catalysis, NATO Advanced Research Workshop* (in press).
25. Kraus M.: Substituent effects. Chapter 5.3.1 in *Handbook of Heterogeneous Catalysis* (Eds. J. Ertl, H. Knözinger, J. Weitkamp), Verlag Chemie, Weinheim, Vol. 3, 1051-1064 (1997).
26. Kraus M.: Dehydrogenation of Alcohols. Chapter 4.3.3 in *Handbook of Heterogeneous Catalysis* (Eds. J. Ertl, H. Knözinger, J. Weitkamp), Verlag Chemie, Weinheim, Vol. 5, 2159-2165 (1997).
27. Kraus M.: Elimination and addition reactions. Chapter 4.8 in *Handbook of Heterogeneous Catalysis* (Eds. J. Ertl, H. Knözinger, J. Weitkamp), Verlag Chemie, Weinheim, Vol. 5, 2370-2380 (1997).

#### Conferences

28. Cinibulk J., Vít Z.: Hydrodenitrogenace pyridinu a hydrodesulfurizace thiofenu na iridiových katalyzátorech. (Czech) HDN of pyridine and HDS of thiophene over Ir catalysts. 24. konferencia SSCHI, Zborník p. 313, Častá-Papiernička, Slovakia, 15-19 June (1997).
29. Čápek P., Hejtmánek V., Šolcová O., Schneider P.: Vznik tlakového rozdílu při vícesložkovém transportu plynů v porézní pevné látce. (Czech) The pressure difference during multicomponent gas transport in porous material. 24. konferencia SSCHI, Zborník p. 351, Častá-Papiernička, Slovakia, 15-19 June (1997).
30. Čápek P., Hejtmánek V., Šolcová O., Schneider P.: Dynamic transport of adsorbable gases in porous catalyst. XXIX. Symposium on Catalysis, Sborník Po 6, Praha, 3-4 November (1997).
31. Frimmel J., Zdražil M.: Paralell hydrodechlorination of dichlorobenzene and hydrodesulphurization of methylthiophene over carbon supported transition metal sulphides.

- Third European Congress on Catalysis EuropaCat-3, Abstr., Vol. 2, p. 543, Kraków, Poland, 31 August - 6 September (1997).
32. Galíková A., Galík A.: Studium adsorpce propylaminů na alumině pomocí mikrovah CAHN D200. (Czech) The study of adsorption of propylamines on alumina using microbalance CAHN D200. 24. konferencia SSCHI, Zborník pp. 161-164, Častá-Papiernička, Slovakia, 15-19 June (1997).
  33. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. Third European Congress on Catalysis EuropaCat-3, Abstr. Vol. 1, 85, Kraków, Poland, 31 August - 6 September (1997).
  34. Kostova N. G., Spojakina A. A., Jiráťová K., Dimitrov L. D., Petrov L. A.: Hydrogenolysis of thiophene on zirconium containing hexagonal mesoporous silicates. 4th National Conference of Bulgarian Catalysis Club, Sofia, 22-23 October (1997).
  35. Kostova N. G., Spojakina A. A., Savova D. N., Jiráťová K.: Effect of support on properties of molybdenum containing catalysts for hydrogenolysis. 4th National Conference of Bulgarian Catalysis Club, Sofia, 22-23 October (1997).
  36. Kostova N. G., Spojakina A. A., Savova D. N., Jiráťová K.: H-irradiation effect on hydrodesulphurization activity of molybdenum containing catalysts. Third European Congress on Catalysis EuropaCat-3, Abstr., Vol. 2, p. 572, 31 August - 6 September (1997).
  37. Ponec R.: Pair population analysis. A new means of analysis and visualisation of molecular structure. 7th International Conference on Mathematical Chemistry, p. 42, Girona, Spain, 26-31 May (1997).
  38. Ponec R.: Similarity approach to chemical reactivity: spin recoupling in chemical reactions. 12th Dubrovnik International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Science, Dubrovnik, Croatia, 23-28 June (1997).
  39. Šolcová O., Hejtmánek V., Šnajdaufová H., Schneider P.: Difuze a adsorpce v plněné chromatografické koloně (SPSR). (Czech) Diffusion and adsorption in the chromatographic column. 24. konferencia SSCHI, Zborník p. 159, Častá-Papiernička, Slovakia, 15-19 June (1997).
  40. Tupý J., Ponec R.: Pair populations and quantitative measures of molecular similarity. 7th International Conference on Mathematical Chemistry, p. 106, Girona, Spain, 26-31 May (1997).
  41. Vít Z.: Stoichiometry of reaction between MoO<sub>3</sub> and OH groups of alumina. III. European Congress on Catalysis, Kraków, Poland, 31 August - 6 September (1997).
  42. Cinibulk J., Vít Z.: HDN of pyridine and HDS of thiophene over Ir catalysts. XXIX. Symposium on Catalysis, Praha, Sborník Po 5, 3-4 November (1997).

## Department of Multiphase Reactors

Head: J. Drahoš  
Deputy: J. Zahradník  
Research staff: M. Fialová, V. Pěnkavová, M. Punčochář, J. Slezák, M. Růžička, V. Sobolík,  
J. Tihon, O. Wein, J. Wichterlová, K. Wichterle  
Part time: P. Mitschka, J. Vrba  
Technical staff: S. Nováková, A. Zemek (part time)  
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

#### Fuzzy models and fractal structures

(M. Punčochář)

Fuzzy sets theory is applied to modelling of complex technological processes. Relation between uncertainty and geometrical complexity is studied using fractal geometry analysis. [Refs. 7, 11, 12, 16]

#### Resources recycling in Eastern Europe

(M. Punčochář, joint project with National Institute of Resources and Environment, Tsukuba, Japan; supported by Ministry of International Trade and Industry, Japan)

The aim of the project is elaboration of the methodological know-how for treatment of industrial solid waste with main impact on recycling of heavy metals.

#### 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  $k$ - $\epsilon$ , RNG and RSM models of turbulent flow in agitated systems from local velocity distributions measured by using the Laser-Doppler anemometry and electrodiffusion diagnostics.

### **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 velocity gradients is measured by simple and segmented electrodiffusion probes.

### **Study of Taylor-Couette instability using three-segment electrodiffusion probe**

(V. Sobolík, supported by GA CR, grant No. 104/95/0654)

Both azimuthal and axial components of the shear rate were measured by means of a recently developed three-segment electrodiffusion probe, flush-mounted in the wall of the outer steady cylinder. The axial dependence of these components was scanned by sweeping the vortices along the probe by superposed slow axial flow. [Refs. 8, 9, 14, 35, 36]

### **Electrochemical sensors for flow measurements**

(V. Sobolík, COST project supported by the Ministry of Education, OC G3.10 (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. 1, 37]

### **Transport phenomena in impinging jet**

(V. Sobolík, joint project with CTU, Faculty of Mechanical Engineering; supported by GA CR, grant No. 101/95/1421)

Mass transfer and shear rate in the vicinity of the stagnation point in an impinging jet have been studied using the electrodiffusion diagnostics. Comparison has been made with numerical solutions and experimental results obtained by naphthalene method.

### **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. 2, 33, 38]

### **New polymers; determination of oxygen permeability**

(K. Wichterle, joint project with PICT and Inst. Macromol. Chem. ASCR; supported by GA CR, grant No. 203/95/1146)

Transient and steady state mass transfer in the material was examined using the cathodic reduction of oxygen on golden electrodes. A new technique employing this principle has been developed for the evaluation of oxygen permeability, diffusion coefficient, and oxygen solubility in new, fluor-containing biocompatible materials.

### **Electrodiffusion diagnostics of high shear rate flows**

(K. Wichterle, supported by GA ASCR, grant No. A4072502)

Extremely high shear rates in liquids have been realized on high speed rotating bodies. Results of the electrodiffusion measurements correspond with laminar boundary layer theory even at high Reynolds numbers and can also be used for investigation of the effect of turbulence. The method was applied in the research of shear rates in centrifugal pumps. Solution of a number of related unsteady state flow and mass transfer problems provided a theoretical background to the method.

[Refs. 8, 9, 14, 22, 30]

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

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

Experimental study proved significant differences in gas phase mixing and in the rate of mass transfer between coalescent and non-coalescent liquid batches. Values of the liquid-side volumetric mass transfer coefficient  $k_L a$  measured in the ejector and in the reactor vessel reflected large intensity of mass transfer in the ejector. The differences between  $k_L a$  data for the two respective reactor zones were, however, significantly less pronounced in non-coalescent systems. [Refs. 3, 15, 25]

### **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).

Experimental programme has been primarily aimed at examining the effect of design and working parameters of bubble column reactors on the formation and stability of the homogeneous and the heterogeneous bubbling regimes in these reactors and at identifying the effect of bubbling regime transition on the hydrodynamic and mass transfer characteristics of gas-liquid beds. In addition, an experimental study proved that behaviour of viscous aerated batches in bubble column reactors can be, in a wide region, modified by small amounts of surface active additives. [Refs. 5, 10, 32, 40, 41]

## **International cooperations**

University of Tokyo, Tokyo, Japan: Chaotic hydrodynamics of bubble columns  
 Hokkaido University, Sapporo, Japan: Processing of coal sorbents containing heavy metals  
 University of Sao Paulo, Brazil: Neural network in prediction of hydrodynamic regimes  
 University of Birmingham, Birmingham, UK: Multiphase chemical reactors and bioreactors  
 UMIST, Manchester, UK: Gas-liquid reactors for complex rheology fluids  
 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  
 Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria: Gas-liquid reactors for complex rheology fluids

## Visits abroad

J. Drahoš: Kyoto University, Kyoto, Japan; University of Helsinki, Helsinki, Finland; Technion, Haifa, Israel; Tel-Aviv University, Tel-Aviv, Israel; University of Hannover, Hannover, FRG  
M. Růžička: University of Birmingham, Birmingham, UK; UMIST Manchester, UK  
V. Sobolík: University of Munich, Munich, FRG; CNRS UPR 15, Paris, France  
J. Tihon: CNRS UPR 15, Paris, France (3 months)  
J. Zahradník: University of Birmingham, Birmingham, UK; UMIST Manchester, UK

## Visitors

H. Iwata, NIRE, Tsukuba, Japan  
T. Chiba, J. Hayashi, Hokkaido University, Sapporo, Japan  
R. Mann, UMIST Manchester, UK  
D. S. Vlaev, UMIST Manchester, UK  
V. Tovchigrechko, ITMO Minsk, Byelorussia (12 months)  
C. Deslouis, CNRS, UPR 15, Paris, France  
R. de Korte, TU Delft, Delft, Netherlands - PhD student  
N. Ravn, Technical University of Denmark, Lyngby, Denmark - IAESTE student  
E.-K. Stenskrog, Technical University of Denmark, Lyngby, Denmark - student (3 months)

## Teaching

J. Drahoš: PICT, course "Fluid Mechanics"  
J. Drahoš: PICT, postgraduate course "Applied Statistical Analysis and Data Processing"  
K. Wichterle: TU Ostrava, courses "Process Engineering", "Transport Phenomena", "Reactor Engineering", "Physical Chemistry of Combustion" and "Chemical Technology"  
O. Wein: TU Brno, course "Principles of Rheology"  
J. Zahradník: PICT, postgraduate course "Multiphase Reactors"

## Publications

### Papers

1. Bewersdorf H.-W., Gyr A., Hoyer K., Sobolík V.: Simultaneous wall shear rate measurements by a three-segment electrodiffusion probe and laser-Doppler-anemometry. *Exp. Fluids* 22, 281-285 (1997).
2. Drahoš J., Tihon J., Sobolík V., Hasal P., Schreiber I., Marek M.: Analysis of wave modes in liquid film falling down a vertical oscillating plate. *Chem. Eng. Sci.* 52, 1163-1176 (1997).



3. Havelka P., Linek V., Sinkule J., Zahradník J., Fialová M.: Effect of the ejector configuration on the gas suction rate and gas hold-up in ejector loop reactors. *Chem. Eng. Sci.* 52, 1701-1713 (1997).
4. Kikuchi R., Yano T., Tsutsumi A., Yoshida K., Punčochář M., Drahoš J.: Diagnosis of chaotic dynamics of bubble motion in a bubble column. *Chem. Eng. Sci.* 52, 3741-3745 (1997).
5. Mann R., Vlaev D., Lossev V., Vlaev S. D., Zahradník J., Seichter P.: A network-of-zones analysis of the fundamentals of gas-liquid mixing in an industrial stirred bioreactor. *Recent Prog. Genie Proc.* 11, 223-230 (1997).
6. Růžička M., Drahoš J., Zahradník J., Thomas N. H.: Intermittent transition from bubbling to jetting regime in gas-liquid two phase flows. *Int. J. Multiphase Flow* 23, 671-682 (1997).
7. Vrba J., Punčochář M., Drahoš J.: Formal uncertainty and membership transfer in fuzzy simulation of complex technological systems. *SAMS* 28, 43-67 (1997).
8. Wein O., Sobolík V.: Dynamics of electrodiffusion friction probes. I. Shape-dependent potentiostatic transient. *Collect. Czech. Chem. Commun.* 62, 397-419 (1997).
9. Wein O., Sobolík V., Tihon J.: Dynamics of electrodiffusion friction probes. II. Shape-dependent impedance. *Collect. Czech. Chem. Commun.* 62, 420-441 (1997).
10. Zahradník J., Fialová M., Růžička M., Drahoš J., Kašánek F., Thomas N. H.: Duality of the gas-liquid regimes in bubble column reactors. *Chem. Eng. Sci.* 52, 3811-3826 (1997).
11. Punčochář M., Drahoš J.: Fractal geometry: A tool for fuzzy reasoning. *Int. J. General Systems* (in press).
12. Punčochář M., Vrba J., Drahoš J.: Membership function for modelling of hierarchical processes. *SAMS* (in press).
13. Růžička M.: On bubbles rising in line. *J. Fluid Mech.* (in press).
14. Sobolík V., Tihon J., Wein O., Wichterle K.: Calibration of electrodiffusion friction probes using voltage-step transient. *J. Appl. Electrochem.* (in press).
15. van Dierendonck L. L., Zahradník J., Linek V.: Loop Venturi reactor - a feasible alternative to stirred tank reactors. *Ind. Eng. Chem. Res.* (in press).
16. Vrba J.: Mass transfer models with fuzzy parameters. *Int. J. Syst. Anal. Model. Simul.* (in press).
17. Vrba J.: Recycle processes - costs analysis and optimization. *SAMS* (in press).
18. Vrba J.: Recycle processes - a note on the convergency of their sequential steady-state simulation. *SAMS* (in press).
19. Wein O.: Diffusion-layer theory for flows under apparent wall slip. *Collect. Czech. Chem. Commun.* (in press).
20. Wein O.: Apparent wall slip in rotational viscometry. *Rheol. Acta* (in press).
21. Wein O., Wichterlová J., Sobolík V.: Viskozita vodných roztoků polyglykolu EMKAROX HV 45. (Czech) Viscosity of aqueous solutions of EMKAROX HV 45 polyglycole. *Chem. Prum.* (in press).
22. Wichterle K., Mitschka P.: Shear of non-Newtonian liquids in impeller induced flow. *Collect. Czech. Chem. Commun.* (in press).
23. Wichterlová J., Wein O., Kašánek F.: Particle migration in a Helle-Shaw cell with non-parallel walls. *Collect. Czech. Chem. Commun.* (in press).
24. Wichterlová J., Rod V.: Dynamic behaviour of the mixer-settler cascade. Extractive separation of the rare earths. *Chem. Eng. Sci.* (in press).
25. Zahradník J., Fialová M., Linek V., Sinkule J., Řezníčková J., Kašánek F.: Dispersion efficiency of ejector-type gas distributors in different operating modes. *Chem. Eng. Sci.* (in press).

## Monographs

26. Drahoš J., Růžička M., Pěnkavová V., Serio C.: Chaotic dynamics of bubble formation in a pool of liquid. *Fractals and Chaos in Chemical Engineering* (Ed. M. Giona), pp. 397-408, World Scientific, Singapore (1997).
27. Punčochář M., Pekárek V., Stach J.: Průmyslové zdroje halogenovaných organických polutantů a jejich potenciální prevence. (Czech) Industrial sources of halogenated organic pollutants and their possible prevention. *Zpravodaj MŽP* 7, pp. 1-8; MŽP, Konzultační a inženýrské služby v životním prostředí, Praha, pp. 1-31 (1997).
28. Wichterle K.: Povrchové/mezifázové napětí v hydrostatice a hydrodynamice. (Czech) Surface/interfacial tension in hydrostatics and hydrodynamics. *Edice MAPRINT No. 20, Nakl. "Procesní inženýrství"*, p. 1-35 (1997).

#### DrSc. Thesis

29. Wein O.: Transport processes under apparent wall slip effect. *Doktorská disertace, CTU Praha* (submitted).
30. Wichterle K.: Modelování procesů v míchané vsádce. (Czech) Modelling of processes in agitated vessel. *Doktorská disertace, CTU Praha* (1997).

#### Conferences

31. Drahoš J., Růžička M., Pěnkavová V.: Chaotic bubbling in a pool of liquid. *International CFIC 96 Conference "Fractals and Chaos in Chemical Engineering"*, Rome, Italy, 2-5 September (1997).
32. Mann R., Vlaev D., Lossev V., Vlaev S. D., Zahradník J., Seichter P.: A network-of-zones analysis of the fundamentals of gas-liquid mixing in an industrial stirred bioreactor. *9th European Conference on Mixing, Paris, France, 18-21 March* (1997).
33. Pěnkavová V., Tihon J.: Vlnový tok viskoelastických kapalin. (Czech) Wavy film flow of viscoelastic liquids. *24. konferencia SSCHI, Zborník pp. 365-368, Častá-Papiernička, Slovakia, 15-19 June* (1997).
34. Růžička M., Drahoš J., Pěnkavová V.: Dynamika tvorby bublin v systémech plyn-kapalina: vliv cirkulace kapalné fáze. (Czech) Dynamics of bubble formation in gas-liquid systems: influence of liquid phase circulations. *24. konferencia SSCHI, Zborník pp. 209-212, Častá-Papiernička, Slovakia, 15-19 June* (1997).
35. Sobolík V., Slezák J.: Study of Taylor-Couette flow using electrodiffusion method. *Workshop Varna'97 "Transport Phenomena in Two-Phase Flow"*, pp. 30-31, Varna, Bulgaria, 12-17 September (1997).
36. Sobolík V., Benabes B., Cognet G.: Velocity gradient distribution at the outer wall of Couette-Taylor flow. *10th International Couette-Taylor Workshop*, p. 145, Paris, France, 15-18 July (1997).
37. Tihon J.: Recirkulační proudění kapaliny v kanále za náhlým rozšířením. (Czech) Recirculation backward-facing step flows. *24. konferencia SSCHI, Zborník pp. 597-600, Častá-Papiernička, Slovakia, 15-19 June* (1997).
38. Tihon J., Pěnkavová V., Sobolík V., Drahoš J.: Wavy film flow of viscoelastic liquid along an inclined plane. *Workshop Varna'97 "Transport Phenomena in Two-Phase Flow"*, pp. 25-26, Varna, Bulgaria, 12-17 October (1997).
39. Veselý V., Punčochář M., Drahoš J.: Vliv spalovacího režimu na tvorbu organických polutanů na popílčích. (Czech) Effect of combustion regime on the formation of organic pollutants on flying ashes. *24. konferencia SSCHI, Zborník pp. 29-32, Častá-Papiernička, Slovakia, 15-19 June* (1997).

40. Vlaev S. D., Mann R., Vlaev D., Lossev V., Zahradník J., Seichter P.: Fundamentals of gas-liquid mixing in an industrial Thylosin reactor. 16th Biennial North American Mixing Conference, Williamsburg, Virginia, USA, 22-27 June (1997).
41. Zahradník J., Kuncová G., Fialová M.: Vliv povrchově aktivních látek na koalescenci bublin a zadrž plynů ve viskózních probublávaných vsádkách. (Czech) The effect of surface active substances on bubble coalescence and gas hold up in viscous aerated batches. 24. konferencia SSCHI, Zborník pp. 505-508, Častá-Papiernička, Slovakia, 15-19 June (1997).

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### Fields of research

- Aerobic bioreactor with immobilized cells - design and scale-up
- Immobilization of biomaterials by sol-gel technique
- Bioremediation of organic pollutants in waste waters
- Detoxification of noxious halogen-containing substances by chemical and biochemical dehalogenation
- Optical fibre sensors for chemical reactors, monitoring of water and soil pollution
- Microwave-induced chemical reactions
- Catalysis by organometallic complexes in aqueous systems
- Immobilization of biocatalysts, development of new agents for their chemical bonding to inorganic supports
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals

### Applied research

- Pilot-scale sorption and biodegradation of PCBs from ground water, performed on an equipment with capacity of 10 m<sup>3</sup> per day
- Hydrogenation of low molecular weight telechelic polybutadienes

### Research projects

#### Catalysts for hydrogenation of lipids in cell membranes

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

Surface area of pentamethylcyclopentadiene-functionalized polysiloxanes prepared by a sol-gel process was found to be controllable by the amount of the functionalizing agent in the starting mixture of alkoxysilanes. Rhodium complexes with alkoxysilyl anchoring groups were synthesized, and polysiloxanes prepared from them exhibited catalytic activity in hydrogenation of crotonic acid in aqueous medium.

**Environmental biotechnology and environmental chemical engineering**

(F. Kaštánek, joint project with PICT)

The mechanism of extraction and emulsification of organic liquids including polychlorinated biphenyls and chlorinated ethenes from soil into an aqueous phase was studied. Various types of natural and synthetic tensides were designed to increase the availability of the organic phase for biocatalysts. The investigation of degradation pathways of the above-mentioned organic compounds brought new information on natural and controlled reductive dechlorination of PCBs in the presence of various hydrogen transfer agents. The dechlorination mechanisms of particular PCB congeners were determined. [Refs. 18, 20, 35]

**Structure of carp gonadotrophin and its bioactivity**

(J. Hetflejš, joint project with CU and IOCB, supported by GA CR, grant No. 505/95/0606)

Separation of glycoproteins from unglycosylated proteins was effected with a bio ligand attached to a porous glass support modified with amino groups. The principle and effectiveness of such a separation has been examined for the isolation of gonadotrophins (G+H) from dehydrated carp lypophyses (I. Hálová: PhD thesis, CU 1997).

**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)

The influence of different immobilization techniques, including methods of immobilization by sol-gel technique into organic matrices, on changes of biodegradation activity of microbial population towards aromatic hydrocarbons was evaluated. [Refs. 10, 13, 21-23, 38, 39]

**Dehalogenation of polychlorinated biphenyls by Fenton's reagent**

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

In the initial stage of the study, the conditions for oxidative decomposition of model polychlorinated aromatics, phenols and simple polychlorobiphenyls by hydrogen peroxide catalyzed by Fe(II) salts have been optimized. The analysis of reaction mixtures and product identification has been worked out, especially for complex oxidation of polychlorophenols. A comparative study of the course of hydrogenative degradation of Delor 103 has been performed, using group determination in complex reaction mixture during consecutive dechlorination of different PCB congener groups. [Refs. 15, 42]

**Technology of organic chlorinated pollutants biodegradation**

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

The technology of biological degradation of chlorinated organic compounds was designed and verified experimentally. Microorganisms complying with legislative demands for biodegradation usage are immobilized into mechanically and chemically resistant matrix which enables to achieve the high concentration of microorganisms in the reactor. The course of biodegradation is followed by means of optical methods. [Refs. 18, 20, 35-37]

**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 a strong local superheating microwave effects on solid samples. Temperature gradients (up to 50 °C) were successfully eliminated indicating that no specific activation occurred. In addition to the main project a new activation method of photochemical reactions by microwave irradiation has been developed and a new scientific discipline Microwave Photochemistry has been established. [Refs. 3, 27, 28, 31-33]

### **Catalysis by transition metal complexes with azine ligands**

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

Novel nickel(0) and palladium(0) complexes with bis(diphenylphosphino)pinacolone azine were prepared and characterized by multinuclear NMR spectroscopy and FAB mass spectrometry, the structure of a palladium complex was determined by X-ray diffraction. Electrochemical activation of a coordinated alkyne was possible with the palladium complex. Methallyl palladium(II) and nickel(II) complexes were synthesized and found to undergo an unusual migration of a methylene proton from the ligand backbone to the metal coupled with reductive elimination. Models of SHOP catalysts - phosphinoenolate complexes of nickel(II) and palladium(II) were prepared from diisopropylphosphinopinacolone and characterized. [Refs. 2, 11, 24-26, 29, 30]

### **International cooperations**

Lajos Kossuth University, Debrecen, Hungary: Ligands for biocompatible hydrogenation catalysts

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

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

Institute of Technical Chemistry, University of Hannover, Hannover, FRG: In-situ monitoring of fluorescence in bioreactors

### **Visits abroad**

V. Církvá: Université de Paris-Sud, Paris, France (2 months)

G. Kuncová: University of Birmingham, UK; UMIST Manchester, UK

J. Čermák: Instituto Superior Técnico, Lisbon, Portugal

### **Visitors**

C. Lindeman, T. Pekeler: Institute of Technical Chemistry, University of Hannover, Hannover, FRG

R. Metaxas: University of Cambridge, Cambridge, UK

### **Teaching**

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

### **Publications**

## Papers

1. Čermák Jan, Kvíčalová M., Blechta V.: Nickel(0) and palladium(0) complexes with 1,3,5-triaza-7-phosphaadamantane. Catalysis of butadiene oligomerization or telomerization in an aqueous biphasic system. *Collect. Czech. Chem. Commun.* 62, 355-363 (1997).
2. Čermák Jan, Shaw B. L.: Nickel(II) and palladium(II) phosphinoenolate complexes derived from  $[(\text{CH}_3)_2\text{CH}]_2\text{PCH}_2\text{C}(\text{O})\text{C}(\text{CH}_3)_3$ . *Chem. Listy* 91, 630-631 (1997).
3. Hájek M.: Microwave activation of homogeneous and heterogeneous catalytic reactions. *Collect. Czech. Chem. Commun.* 62, 347-354(1997).
4. Kuncová G., Šivel, M.: Lipase immobilized in organic-inorganic matrices. *J. Sol-Gel Sci. Technol.* 8, 667-671(1997).
5. Kvíčalová M., Blechta V., Kobylczyk K., Piekos R., Schraml J.: Silicon-29 NMR spectra of tert-butyldimethylsilyl and trimethylsilyl derivatives of some non-rigid diols. *Collect. Czech. Chem. Commun.* 62, 761-768 (1997).
6. Kvíčalová M., Čermák Jan, Blechta V., Schraml J.: Silicon-29 NMR spectra of trimethylsilylated alcohols. *Collect. Czech. Chem. Commun.* 62, 816-820 (1997).
7. Schraml J., Kvíčalová M., Blechta V., Čermák Jan:  $^{29}\text{Si}$  NMR spectra of tert-butyldimethylsilylated alcohols. *Magn. Reson. Chem.* 35, 659-662 (1997).
8. Tříška J., Kuncová G., Hayer M.: Křemenné kapilární kolony. (Czech) Quartz capillary columns. *Chem. Prum.* 4, 26 (1997).
9. Zahradník J., Fialová M., Růžička M., Drahoš J., Kaštánek F., Thomas N. H.: Duality of the gas-liquid regimes in bubble column reactors. *Chem. Eng. Sci.* 52, 3811-3826 (1997).
10. Brányik T., Kuncová G., Páca J., Demnerová K.: Encapsulation of microbial cells into silica gel. *J. Sol-Gel Sci. Technol.* (in press).
11. 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).
12. Schraml J., Kvíčalová M., Blechta V., Řeřicha R., Rozenski J., Herdewijn P.:  $^{29}\text{Si}$  NMR spectra of trimethylsilyl and tert-butyldimethylsilyl derivatives of purines and pyrimidines. *Magn. Reson. Chem.* (in press).
13. 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.* (in press).
14. Šmíd J., Včelák J., Hanykýř V.: Messglied eines Gebers fuer die Ermittlung von Normal- und Tangentialspannungen keramischer Gemische. (Ger) Dynamometric element of the pressure cell for measuring the normal and tangential stresses of ceramic mixture. *SPRECHSAAL - Int. Ceram. Glass Mag.* (in press).
15. Včelák J., Hetflejš J.: Catalytic dehalogenation of PCB waste by complex hydrides. *Chemosphere* (in press).
16. Wichterlová J., Wein O., Kaštánek F.: Particle migration in a Helle-Shaw cell with non-parallel walls. *Collect. Czech. Chem. Commun.* (in press).
17. Zahradník J., Fialová M., Linek V., Sinkule J., Řezníčková J., Kaštánek F.: Dispersion efficiency of ejector-type gas distributors in different operating modes. *Chem. Eng. Sci.* (in press).

## Monographs

18. Kaštánek F., Demnerová K.: Biodegradation of alkanes and PCB: Experience in the Czech Republic. Adv. Research Symposium Series NATO, Springer Verlag (1997).
19. Punčochář M., Pekárek V., Stach J.: Průmyslové zdroje halogenovaných organických polutantů a jejich potenciální prevence. (Czech) Industrial sources of halogenated organic pollutants and their possible prevention. Zpravodaj MŽP 7, pp. 1-8; MŽP, Konzultační a inženýrské služby v životním prostředí, Praha, pp. 1-31 (1997).
20. Demnerová K., Burkhard J., Kaštánek F., Košťál J., Kuncová G., Macek T., Macková M., Pazlarová J.: Biodegradation of alkanes and PCBs: Experience in the Czech Republic. In: NATO ASI Series, Kluwer, Dordrecht, pp. 53-70 (1997).

#### Conferences

21. Brányik T., Kuncová G., Páca J., Jurek K.: Encapsulation of microbial cells into silica gel. 9th International Workshop on Glasses, Ceramics, Hybrids and Nanocomposites from Gel, Abstr. CP 9, Sheffield, UK, 31 August-5 September (1997).
22. Brányik T., Kuncová G., Páca J.: The influence of encapsulation of microbial cells on phenol degrading activity. Comparison of silica gel and polyurethane. Proc. of Int. Workshop Bioencapsulation VI, P. 38, Barcelona, Spain, 30 August-1 September (1997).
23. Brányik T., Kuncová G., Páca J.: Polyurethane as immobilization material for phenol degradation. Comparison of entrapment and adsorption of cells. ISEB'97-Meeting Bioremediation, Abstr. p. 102, Leipzig, FRG, 24-27 September (1997).
24. Carvalho M. F. N. N., Čermák Jan, Herrmann R., Pombeiro A. J. L., Wagner G.: Activation of unsaturated carbon-carbon or carbon-nitrogen bonds in ligands coordinated at electron-rich metal centers. 4th FGIPS Meeting in Inorganic Chemistry, Abstr. p. MLB 3, Corfu, Greece, 14-18 August (1997).
25. 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. Portuguese Electrochemistry Meeting, Abstracts, Braga, Portugal, 17-20 September (1997).
26. Carvalho M. F. N. N., Čermák Jan, Šabata S., Duarte M. T., Francisco F. A., Galvao A. M., Pombeiro A. J. I.: Alkyne to vinyl conversion induced by electron transfer. X-ray structure of  $\text{trans-[Pd}\{\text{PPh}_2\text{CH=C(But)NN=C(But)CH}_2\text{PPh}_2\}\text{C(CO}_2\text{Me)=C(H)CO}_2\text{Me}]$ . XIIth FEICHEM Conference on Organometallic Chemistry, Abstracts p. PA136, Praha, 31 August - 5 September (1997).
27. Církva V., Hájek M.: Microwave photochemistry in organic synthesis. Microwave and High Frequency Heating, Proc. pp. 153-156, Fermo, Italy, 9-13 September (1997).
28. Církva V., Hájek M.: New formation of aryl carbon-phosphorus bonds. XIIth Conference of Organic Chemists on Advances in Organic Chemistry, Proc. p. 139, Častá-Papiernička, Slovakia, 11-13 June (1997).
29. Čermák Jan, Shaw B. L.: Reaction of  $[(\text{CH}_3)_2\text{CH}]_2\text{PCH}_2\text{C(O)C(CH}_3)_3$  with nickel (0) and palladium(II) complexes - Models of SHOP catalysts. 9th IUPAC Symposium on Organometallic Chemistry Directed towards Organic Synthesis, Abstracts p. 516, Gottingen, FRG, 21-25 July (1997).
30. Čermák Jan, Blechta V., Shaw B. L.: 2-Methylallylnickel(II) complexes with an azine diphosphine ligand,  $\text{Ph}_2\text{PCH}_2\text{C(But)=NN=C(But)CH}_2\text{PPh}_2$ . XIIth FEICHEM Conference on Organometallic Chemistry, Abstracts p. PA138, Praha, 31 August - 5 September (1997).
31. Hájek M.: Application of microwave energy in catalysis. Short course on principles and application of microwave and high frequency heating, educational approach p. 85, Fermo, Italy, 9-13 September (1997).



32. Hájek M., Richterová H.: Local microwave heating effects in liquid and solid state chemistry. Microwave and High Frequency Heating, Proc. pp. 79-81, Fermo, Italy, 9-13 September (1997).
33. Hájek M., Richterová H., Stach J.: Microwave enhanced organic reactions. XIIth Conference of Organic Chemists on Advances in Organic Chemistry, Proc. pp. 148-149, Častá-Papiernička, Slovakia, 11-13 June (1997).
34. Havránek V., Kučera J., Kolman B., Kugler J., Pekárek V., Schwarz J., Smolík J., Výška J., Příbyl J.: Effect of fuel on particle from gasoline powered vehicle. European Aerosol Conference, Hamburg, 15-19 September, J. Aerosol Sci. 28(S1), 547-548 (1997).
35. Kaštánek F., Demnerová K.: Fate of waste chlorinated alkanes and PCB in the environment. Symp. of industrial microbiology, Am. Soc. of Microbiology, Reno, USA, August (1997).
36. Kotlíková J., Kuncová G., Burkhard J., Klepaczová I., Paznerová J., Demnerová K., Pazlarová J.: Biodegradation of PCBs by free and immobilised bacterial cells. Advanced Study Institute: Bioavailability of organic xenobiotic in the environment, p. 87, Jeseník, Czech Republik, 18-29 August (1997).
37. Kotlíková J., Kuncová G., Burkhard J., Paznerová J., Demnerová K., Pazlarová J.: Biodegradation of polychlorinated biphenyls by immobilized cells. Mini-Symposium on Biosorption and Microbial Degradations, Abstracts, Praha, 24-28 November (1997).
38. Marek J., Páca J., Kuncová G.: Microbial degradation of phenol in packed bed reactors. ISEB '97 Meeting Bioremediation, Abstracts p. 102, Leipzig, FRG, 24-27 September (1997).
39. Szilva J., Kuncová G., Patzák M., Dostálek P.: The application of sol-gel technique for preparation of heavy metal biosorbent from yeast cells. 9th International Workshop on Glasses, Ceramics, Hybrids and Nanocomposites from Gels, Abstr. CP 10, Sheffield, UK, 31 August-5 September (1997).
40. Zahradník J., Kuncová G., Fialová M.: Vliv povrchově aktivních látek na koalescenci bublin a zadrž plynu ve viskózních probublávaných vsádkách. (Czech) The effect of surface active substances on bubble coalescence and gas hold up in viscous aerated batches. 24. konference SSCHI, Zborník pp. 505-508, Častá-Papiernička, Slovakia, 15-19 June (1997).
41. Včelák J., Hetflejš J., Czakóová M.: Ru-phospine complexes as catalysts for cinnamaldehyde hydrogenation-selectivity effects. XIIth FEICHEM Conference on Organometallic Chemistry, Abstr. PB 10, Praha, 31 August - 5 September (1997).
42. Hetflejš J.: Odpady s PCB - principy jejich zneškodnění. (Czech). PCB wastes - principles of their disposal. Int. Conference and Exhibition Odpady-Waste-Abfaelle 97, Lectures pp. 44-45, Praha, 10-12 June (1997).

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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 [Refs. 46, 66]

### Research projects

#### Power combustion of wastes and biomass

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

A new 100 kW circulating fluidized bed reactor with modular structure has been built. The effect of combustion regime on the formation of organic pollutants on flying ashes with attention to the evolution of PCDD/F precursors has been explored [Ref. 66]. The experiments with PVC combustion have been done with the aim of determining the efficiency of limestone as sorbent for dropping of PCDD/F emissions.

**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. 3, 28, 29]

**Emission fluxes of heavy metals in the fluidized bed combustion of fossil fuels**

(J. Smolík, supported by GA CR, grant No. 104/95/0653)

The project represents both the experimental and theoretical effort aimed at solving important relationships in the complex processes of combustion, formation and behaviour of metal pollutants within a fluidized bed and in flue gas cleaning units. Special attention has been paid to the mechanism of formation of ultrafine particles enriched by toxic elements and organic pollutants. Main part of the measuring device was acquired, and the experimental apparatus has been built up. [Refs. 16, 17, 21, 57, 59, 60, 63, 64]

**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.

**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. [Refs. 3, 43]

**Fuel reactivity and release of pollutants**

(K. Svoboda, supported by the EC in the program PECO: JOU II-CT 92-0037)

A unique experimental facility with a pressurized fluidized bed has been constructed. The dependence of the NO<sub>x</sub> and N<sub>2</sub>O emissions released by combustion in the pressurized fluidized bed have been explored as to such factors as operating conditions (temperature, excess air, pressure) and types of functional bonds of nitrogen in the liquid or solid fuel. [Refs. 61, 62]

**Studies of atmospheric chemistry and air pollution**

(J. Pola, joint project with the Hebrew University of Jerusalem; supported by the Agency for International Development, Washington, USA, grant No. HRN 5544G00207 and GA CR, grant No. 104/96/0472)

Initial studies on reaction of ozone with 1-hexene at ppm level in nitrogen atmosphere and air have been carried out to identify the products at different temperatures. The studies are to be extended to other olefins. [Refs. 4, 26]

**Laser chemistry of organosilicon compounds for preparation of novel materials**

(J. Pola, supported by GA ASCR, grant No. A 407 2509)

Laser induced decomposition of various organosilicon compounds in the gas phase has been carried out to generate, for the first time, very unsaturated organosilicon transients (bis-(ethynyl)silene, ethenylsilene, methyl(hydroxy)silylene, chlorosilyne, etc.) which undergo very

efficient polymerization. The technique is a unique approach for CVD of novel organosilicon materials with potential application in microelectronics and catalysis. [Refs. 10, 12, 20, 25, 32]

### **Deposition of SiO<sub>2</sub> and Si<sub>2</sub>O/H films from the gas phase**

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

Laser induced chemical vapor deposition was revealed to be a very efficient way of preparation of novel materials containing silicon. SiO<sub>2</sub> and Si<sub>2</sub>O/H films from different organosilicon compounds (e.g., disiloxane) are materials with potential applications as semi-conductors. [Ref. 1]

### **Laser induced silica-derivatization of fullerenes**

(J. Pola, supported by NATO, program KONTAKT, grant No. ES 019 (1996))

Investigation of reactions of different silacyclobutanes (substituted at silicon with aromatic ring, methyl group and hydrogen) with C<sub>60</sub>, induced by IR- and UV-lasers or thermally, is a very promising way of preparing fullerene-containing solid thin films for various applications. [Refs. 9, 39, 44]

### **Mass transfer from evaporating droplet**

(J. Schwarz, supported by GA ASCR, grant No. A 4072504)

A new mass transfer correlation based on a new definition of the Sherwood number has been proposed including mass transfer due to non-isothermal diffusion, radial efflux of vapour, and thermal diffusion. The effect of individual contributions to the mass transfer was investigated during the evaporation of 1-hexanol droplets [Refs. 42, 56]. The facility has also been used for studies on droplet evaporation in the presence of condensable species [Refs. 15, 58].

### **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. During the first year of the project, homogeneous nucleation rates of n-pentanol were studied with helium as an inert gas. [Refs. 47, 67, 68]

## **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

The Hebrew University of Jerusalem, Israel: Studies of atmospheric chemistry and air pollution

Sussex University, Brighton, UK: Sila-derivatization of fullerenes

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

Bhabha Atomic Research Centre, Bombay, India: Laser-induced chemistry

Institute of Petrochemical Synthesis, Moscow, Russia: Laser decomposition of silacycles

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: Chemical vapour deposition of polymeric films

Hokkaido University, Sapporo, Japan: Chlorination of ashes

### Visits abroad

M. Hartman: Dechema, Achema, Frankfurt/M., FRG

J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (1 month); Bhabha Atomic Research Centre, Bombay, India; Bergische Universität, Wuppertal, FRG (1 month); University of Crete, Heraklion, Greece

J. Schwarz: University of Helsinki, Finland (1 month); Finnish Meteorological Institute, Helsinki, Finland (2 months); KAIST, Taejon, Korea

K. Svoboda: Abo Akademi, Turku, Finland

### Visitors

G. I. Kuzmina: Institute of Petrochemical Synthesis, Moscow, Russia (3 months)

E. A. Volnina: Institute of Petrochemical Synthesis, Moscow, Russia (3 months)

R. Hillamo: Finnish Meteorological Institute, Helsinki, Finland

Y. Viisanen: Finnish Meteorological Institute, Helsinki, Finland

T. Chiba: Hokkaido University, Sapporo, Japan

### Publications

#### Papers

1. Dřínek V., Bastl Z., Šubrt J., Pola J.: IR laser induced CVD of SiO<sub>2</sub> phases from triethoxysilane and tetraethoxysilane. *Appl. Surf. Sci.* 108, 283-288 (1997).
2. Hartman M., Trnka O., Beran Z.: Kinetics of the thermal decomposition of hydrated dolomitic lime and sintering of nascent calcine. *Chem. Eng. Commun.* 162, 199-214 (1997).
3. Hartman M., Beran Z., Veselý V., Svoboda K.: On the transition from homogeneous to bubbling fluidization. *Collect. Czech. Chem. Commun.* 62, 1698-1709 (1997).
4. Khachatryan L., Haas Y., Pola J.: Laser-induced decompositions of 3,5-dimethyl-1,2,4-trioxolane (secondary butene-2-ozonide) in the gas phase. *J. Chem. Soc., Perkin Trans.* 1147-1151 (1997).

5. Levdanskij V. V., Moravec P., Smolík J.: Khimicheskoe osazhdenie veshchestva v sisteme gas-aerozol'nye chastitsy. (Russ) Chemical deposition of substances in the system gas-aerosol particles. *Vestsi Akad. Navuk Belarusi, Ser. Fiz.-Tekh. Navuk* 4, 132 (1997).
6. Moravec P., Smolík J., Levdansky V. V.: Nano-sized particles from the CO<sub>2</sub> laser assisted decomposition of tetraethylorthosilicate vapour. *J. Matt. Sci. Lett.* 16, 648-651 (1997).
7. Pola J.: Laser-generated silenes and their gas-phase polymerization. *Radiat. Phys. Chem.* 49, 151-154 (1997).
8. Pola J., Koga Y., Ouchi A.: Laser pyrolysis of 2-propanone, 2-butanone, 3-pentanone and 3-buten-2-one in the gas phase. *Tetrahedron* 53, 3757-3766 (1997).
9. Pola J., Urbanová M., Bastl Z., Plzák Z., Šubrt J., Vorlíček V., Gregora I., Crowley C., Taylor R.: Laser photolysis of liquid benzene and toluene: graphitic and polymeric carbon formation at ambient temperature. *Carbon* 35, 605-661 (1997).
10. Pola J., Morita H.: UV laser induced gas-phase polymerization of trimethyl(2-propynyloxy)silane. *Tetrahedron Lett.* 38, 7809-7812 (1997).
11. Pola J., Pokorná D., Bastl Z., Šubrt J.: IR laser-induced chemical vapour deposition of silicon oxycarbide phases from 1,1,3,3-tetramethyldisiloxane. *J. Anal. Appl. Pyrol.* 38, 153-159(1997).
12. Pola J., Vítek J., Bastl Z., Urbanová M., Šubrt J., Taylor R.: IR laser-induced decomposition of prop-2-enylsilane and ethynylsilane for chemical vapour deposition of Si/C phases. *J. Mater. Chem.* 7, 1415-1420 (1997).
13. Santos M., Díaz L., Torresano J. A., Pola J.: Visible luminiscence study of the infrared multiphoton dissociation of 2-chloroethenylsilane. *J. Photochem. Photobiol.* 104, 19-23 (1997).
14. Smolík J., Moravec P.: Gas phase synthesis of fine silica particles in a tube reactor. *Ceramics (Silikáty)* 41, 7-11 (1997).
15. Smolík J., Schwarz J.: Heterogeneous nucleation of naphthalene vapor on water surface. *J. Colloids Interface Sci.* 185, 382-389 (1997).
16. Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Kučera J.: Tuhé emise z fluidního spalování hnědého uhlí. (Czech) Solid emissions from the fluidized bed combustion of brown coal. *Ochrana ovzduší* 9, 18-21 (1997).
17. Sýkorová I., Šrein V., Šťastný M., Smolík J., Schwarz J., Kučera J., Havránek V.: Popílky z fluidního spalování hnědého uhlí. (Czech) Ashes from the fluidized bed combustion of brown coals. *Uhlí-Rudy-Geologický průzkum* 9, 309-314 (1997).
18. Trnka O., Hartman M., Svoboda K.: An alternative semi-implicit Euler method for the integration of highly stiff nonlinear differential equations. *Comput. Chem. Eng.* 21, 277-282 (1997).
19. Vatsa R. K., Kumar A., Naik P. D., Upadhyay H. P., Pavanaja U. B., Saini R. D., Mittal J. P., Pola J.: UV spectrum and decay kinetics of transient methylsilene produced in the 193 nm photolysis of gaseous methylsilacyclobutane. *Chem. Phys. Lett.* 255, 129-133(1997).
20. Volnina E. A., Kupčík J., Bastl Z., Šubrt J., Guselnikov L. E., Pola J.: Si/C phases from the IR laser-induced decomposition of 1,4-disilabutane. *J. Mater. Chem.* 7, 637-640 (1997).
21. Sýkorová I., Šrein V., Šťastný M., Schwarz J., Smolík J., Veselý V., Kugler J., Kučera J.: Fluidized bed combustion of brown coal from Vrsany mine. *Zesz. Nauk. Politech. Slaskiej, Ser. Gornictwo* 235, 197-203 (1997).
22. Bailleux S., Boggy M., Demaison J., Bürger H., Senzlobler M., Breidung J., Tfiel W., Fajgar R., Pola J.: The equilibrium structure of silene H<sub>2</sub>C=SiH<sub>2</sub> from millimeter wave spectra and from ab initio calculations. *J. Chem. Phys.* 106, 10016-10026 (1997).
23. 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-butyne-2-one. *Carbon* (in press).

24. Dřínek V., Urbanová M., Bastl Z., Gregora I., Vorlíček V., Šubrt J., Pola J.: Carbonaceous phases by IR laser induced decomposition of 3-butyn-2-one. *Appl. Phys. A* (in press).
25. Dřínek V., Bastl Z., Šubrt J., Pola J.: Si/C phases from IR laser-induced decomposition of divinylsilane. *Appl. Organometal.* (in press).
26. Fajgar R., Vítek J., Haas Y., Pola J.: Definitive evidence of the formation of secondary ozonides in the ozonation of alkenes in the gas phase. *J. Am. Chem. Soc.* (in press).
27. Hartman M., Beran Z., Veselý V., Svoboda K.: Particulate and aggregative mode of fluidization. *Chem. Eng. Commun.* (in press).
28. Hartman M., Trnka O., Svoboda K.: Potential of calcium oxide for removal of hydrogen sulphide and carbonyl sulphide from coal gas. *Fuel* (in press).
29. Hartman M., Trnka O., Svoboda K.: Essential factors in removing carbonyl sulphide from coal gas with lime and limestone. *Chem. Eng. Sci.* (in press).
30. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. *Catal. Lett.* (in press).
31. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. Effect of catalyst composition. *React. Kinet. Catal. Lett.* (in press).
32. Khachatryan L., Volnina E. A., Fajgar R., Pola J.: Laser induced decomposition of silacyclobutane: extensive H(Si)/H (C) scrambling via 1,2-H shift in silene and radical reactions. *Organometallics* (in press).
33. Levdanskij V. V., Smolík J., Moravec P., Ždímal V.: O kinetike rosta aerosol'nykh chastits v aerodispersnoi sisteme. (Russ) Kinetics of growth of aerosol particles in aerodispersed system. *Trudy A. V. Luikov HMTI AS RB* (in press).
34. 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).
35. Levdanskij V. V., Moravec P., Smolík J.: Osazhdenie veshchestva iz gazovoi smesi na aerosol'nykh chastitsakh. (Russ) Deposition of substances from gaseous mixture on aerosol particles. *Inzh. Fyz. Zh. (J. Eng. Phys.)* (in press).
36. Levdanskij V. V., Moravec P., Smolík J.: O roste chastic pri khimicheskom osazhdenii veshchestva iz gazovoi fazy, indutsirovannom lazernym izlucheniem. (Russ) On particle growth by laser induced chemical vapor deposition. *Inzh. Fiz. Zh.* (in press).
37. Morita H., Semba K., Bastl Z., Pola J.: Laser-induced aerosol particle formation from a gaseous mixture of trimethyl(2-propynyloxy)silane and acrolein. *J. Photochem. Photobiol.* (in press).
38. Pola J.: Polycarbosilane-based coatings by laser-induced polymerization of silenes in the gas phase. *Surface and Coatings Technol.* (in press).
39. Pola J., Urbanová M., Bastl Z., Plzák Z., Šubrt J., Gregora I., Vorlíček V.: Laser photolysis of liquid hexafluorobenzene: graphitic and fluorine-containing carbon formation at ambient temperature. *J. Mater. Chem.* (in press).
40. Pola J.: UV and IR laser-induced decomposition of organosilanes for CVD of Si/C/H phases. *Radiat. Phys. Chem.* (in press).
41. Smolík J., Moravec P.: Aerosolové procesy pro přípravu práškových materiálů. (Czech) Aerosol processes for powder synthesis. *Silika* (in press).
42. Smolík J., Schwarz J., Kulmala M.: Experimental determination of ventilation coefficient for 1-hexanol drops in air. *Atmos. Res.* (in press).
43. Trnka O., Hartman M.: Behaviour of models of chemical g-s reactions in an ideal mixer with gas velocity fluctuations. *AIChE J.* (in press).

44. 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* (in press).
45. Urbanová M., Morita H., Dřínek V., Bastl Z., Šubrt J., Pola J.: IR laser induced thermal decomposition of trimethyl(2-propynyloxy)silane for chemical vapour deposition of Si/C/O phases. *J. Anal. Appl. Pyrol.* (in press).
46. Veselý V., Hartman M., Svoboda K., Trnka O.: Spalování kapalných paliv ve fluidní vrstvě. (Czech) Incineration of liquid waste in fluidized bed. *Chem. Listy* (in press).
47. Ždímal V., Smolík J.: Homogeneous nucleation rate measurements in 1-pentanol vapor with helium as a buffer gas. *Atmos. Res.* (in press).

### Monographs

48. Svoboda K.: Chemické systémové inženýrství a projektování chemicko-technologických souborů. (Czech) System chemical engineering and chemical process design. Lecture notes, PICT, 225 pp. (1997).

### Conferences

49. Dřínek V., Urbanová M., Pola J.: Laser-induced chemical vapour deposition of carbon-rich glassy phases from 3-butyn-2-one. International Conference on Advanced Materials, Abstr. A-25, Strasbourg, France, 16-20 June (1997).
50. Havránek V., Kučera J., Kolman B., Kugler J., Pekárek V., Schwarz J., Smolík J., Výška J., Příbyl J.: Effect of fuel on particle from gasoline powered vehicle. European Aerosol Conference, Hamburg, 15-19 September, *J. Aerosol Sci.* 28(S1), 547-548 (1997).
51. Jirátová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. Third European Congress on Catalysis EuropaCat-3, Abstr. Vol. 1, 85, Kraków, Poland, 31 August - 6 September (1997).
52. Levanskij V. V., Moravec P., Smolík J.: Aerosol particle growth in process of chemical deposition. European Aerosol Conference, Hamburg, 15-19 September, *J. Aerosol Sci.* 28(S1), 483-484 (1997).
53. Moravec P., Smolík J., Levanskij V. V.: Fine particle synthesis by decomposition of aluminium tri-sec-butoxide vapour. European Aerosol Conference, Hamburg, FRG, 15-19 September, *J. Aerosol Sci.* 28(S1), 481-482 (1997).
54. Morita H., Semba K., Pola J.: Fine particle formation from organic silicone compounds by two-photon process. 17th International Conference on Photochemistry, Abstr. 3P 48, Warsaw, Poland, 3-8 August (1997).
55. Pola J.: Polycarbosilane-based coatings by laser-induced polymerization of silenes in the gas phase. International Conference on Advanced Materials, Abstr. K-23, Strasbourg, France, 16-20 June (1997).
56. Schwarz J., Smolík J.: Mass transfer from evaporating 1-hexanol drop by using two experimental techniques. Proc. 7th Int. Conf. on Liquid Atomization and Spray Systems INCLASS'97, pp. 738-744, Seoul, Korea, 18-22 August (1997).
57. Schwarz J., Smolík J., Veselý V., Kugler J., Sýkorová I., Kučera J., Havránek V.: Aerosol emission from fluidised bed combustion. Short course '97: Metastable behavior and critical phenomena, Praha, 15-16 October (1997).
58. Schwarz J., Smolík J., Vákevä M., Kulmala M., Vesala T.: Studies on droplet evaporation in presence of condensable species. The Sixth Finnish National Aerosol Symposium, pp. 101-103, Helsinki, Finland, 15-16 April (1997).



59. Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Kučera J., Havránek V.: Elemental size distributions of aerosol from combustion of Czech lignites. European Coal Conference'97, pp. 63-64, Izmir, Turkey, 5-10 May (1997).
60. Smolík J., Schwarz J., Veselý V., Kugler J., Sýkorová I., Kučera J., Havránek V.: Matrix and trace element behaviour in fluidized bed combustion of lignite. European Aerosol Conference, Hamburg, 15-19 September, J. Aerosol Sci. 28(S1), 409-410 (1997).
61. Svoboda K., Hartman M., Čermák J.: Emise oxidu dusného ze spalování uhlí. (Czech) Nitrous oxide emissions in coal combustion. 24. konferencia SSCHI, Zborník pp. 23-27, Častá-Papiernička, Slovakia, 15-19 June (1997).
62. Svoboda K., Čermák J., Hartman M., Neužil L.: Dávkování sypkých částic dutými šneky. (Czech) Feeding of particulate materials by hollow screws. 24. konferencia SSCHI, Zborník p. 297, Častá-Papiernička, Slovakia, 15-19 June (1997).
63. Sýkorová I., Šrein V., Šťastný M., Smolík J., Schwarz J., Veselý V., Kučera J.: The reactivity of brown coal in fluidized bed combustion. European Coal Conference'97, pp. 104-105, Izmir, Turkey, 5-10 May (1997).
64. Sýkorová I., Smolík J., Schwarz J., Kerkkonen O., Kučera J., Havránek V.: Composition and morphology of fly ash from fluidized bed combustion of brown coal. 9th International Conference on Coal Science, p. 1187-1190, Essen, FRG, 7-12 September (1997).
65. Urbanová M., Pola J., Bastl Z., Plzák Z., Šubrt J., Vorlíček V.: Laser photolysis of liquid benzene and hexafluorobenzene: graphitic and polymeric carbon formation at ambient temperature. International Conference on Advanced Materials, Abstr. A-25, Strasbourg, France, 16-20 June (1997).
66. Veselý V., Punčochář M., Drahoš J.: Vliv spalovacího režimu na tvorbu organických polutanů na popílcích. (Czech) Effect of combustion regime on the formation of organic pollutants on flying ashes. 24. konferencie SSCHI, Zborník pp. 29-32, Častá-Papiernička, Slovakia, 15-19 June (1997).
67. Ždímal V., Smolík J., Rudek Marcus M., Katz J. L.: Joint experiments on homogeneous nucleation: Static diffusion chamber results. Short course'97: Metastable behavior and critical phenomena, Praha, 15-16 October (1997).
68. Ždímal V., Smolík J., Rudek Marcus M., Katz J. L.: The homogeneous nucleation of n-pentanol in TDCC. European Aerosol Conference, Hamburg, FRG, 15-19 September (1997).

## Department of Analytical Chemistry

Head: J. Schraml  
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### Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

### Applied research

- Analytical services to 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  $^{29}\text{Si}$  NMR are being extended to other fields of NMR to investigate the steric effects in general. [Refs. 6, 8, 9]

#### **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  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{29}\text{Si}$  and  $^{15}\text{N}$  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. [Ref. 2]

### International cooperations

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

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

University of Rostock, Rostock, FRG: Materials for chromatographic separation of enantiomers

Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria: Dynamic NMR

### Visits abroad

J. Schraml: Catholic University of Leuven, Leuven, Belgium; University of Coimbra, Coimbra, Portugal

## Teaching

J. Schraml: CU, course "NMR Spectroscopy"

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

## Publications

### Papers

1. Čermák Jan, Kvíčalová M., Blechta V.: Nickel(0) and palladium(0) complexes with 1,3,5-triaza-7-phosphaadamantane. Catalysis of butadiene oligomerization or telomerization in an aqueous biphasic system. *Collect. Czech. Chem. Commun.* 62, 355-363 (1997).
2. De Bruyn A., Maras M., Schraml J., Herdewijn P., Contreras R.: NMR evidence for a novel asparagine-linked oligosaccharide on cellobiohydrolase I from *Trichoderma reesei* RUTC 30. *FEBS Letters* 405, 111-113 (1997).
3. Kvíčalová M., Blechta V., Kobylczyk K., Piekos R., Schraml J.: Silicon-29 NMR spectra of tert-butyldimethylsilyl and trimethylsilyl derivatives of some non-rigid diols. *Collect. Czech. Chem. Commun.* 62, 761-768 (1997).
4. Kvíčalová M., Čermák Jan, Blechta V., Schraml J.: Silicon-29 NMR spectra of trimethylsilylated alcohols. *Collect. Czech. Chem. Commun.* 62, 816-820 (1997).
5. Maras M., De Bruyn A., Schraml J., Herdewijn P., Claeysens M., Fiers W., Contreras R.: Structural characterization of N-linked oligosaccharides from cellobiohydrolase I secreted by *Trichoderma reesei* RUTC 30. *Europ. J. Biochem.* 245, 617-625 (1997).
6. Schraml J., De Bruyn A., Contreras R., Herdewijn P.: A versatile NMR technique for the identification of phosphorylation sites in oligosaccharides. *J. Carbohydr. Chem.* 16, 165-170 (1997).
7. Schraml J., Kvíčalová M., Blechta V., Čermák Jan: <sup>29</sup>Si NMR spectra of tert-butyldimethylsilylated alcohols. *Magn. Resonan. Chem.* 35, 659-662 (1997).
8. Schraml J., Kvíčalová M., Blechta V., Řeřicha R., Rozenski J., Herdewijn P.: <sup>29</sup>Si NMR spectra of trimethylsilyl and tert-butyldimethylsilyl derivatives of purines and pyrimidines. *Magn. Reson. Chem.* 36, 55-63 (1997).
9. Van Calenbergh S., De Bruyn A., De Keukeleire D., Herdewijn P., Schraml J., Blaton N. M., Peeters O. M.: Access to a new type of homo-C-nucleoside with a "split" 8-deazapurine via a 1,3 dipolar cycloaddition reaction. *Nucleosides Nucleosides* 16, 291-300 (1997).
10. Vohlřídál J., Vangani V. H., Pleček J., Rajabi F. H., Blechta V., Němec I.: Synthesis of new polymers involving deltahedral carborane units. *Macromol. Chem. Phys.* 198, 193-218 (1997).
11. Osson A., De Bruyn A., Schraml J., Herdewijn P., DeKeukeleire D.: A novel polyhydroxylated alkaloidal amine from *solanum elaeagnifolium* with B-glucosidase- and neuraminidase inhibiting activity. A novel polyhydroxylated alkaloidal amine from *solanum*

elaegnifolium with B-glucosidase- and neuraminidase inhibiting activity. FEBS Letters (in press).

12. Sovová H., Komers R., Rat V., Chačaturjan M., Vlček D.: Solubility of squalane and dinonyl phthalate in CO<sub>2</sub> with entrainers. J. Supercrit. Fluids (in press).

#### Conferences

13. Čermák Jan, Blechta V., Shaw B. L.: 2-Methylallylnickel(II) complexes with an azine diphosphine ligand, Ph<sub>2</sub>PCH<sub>2</sub>C(But)=NN=C(But)CH<sub>2</sub>PPh<sub>2</sub>. XIIth FECHEM Conference on Organometallic Chemistry, Abstracts p. PA138, Praha, 31 August - 5 September (1997).
14. De Bruyn A., Schraml J., Maras M., Contreras R., Herdewijn P.: NMR techniques in the study of protein-linked carbohydrates. 9th European Carbohydrate Symposium Eurocarb 9, Utrecht, Netherlands, 6-11 July (1997).
15. Maras M., Laroy W., Saelens X., Martinet W., De Bruyn A., Schraml J., Herdewijn P., Claeysens M., Conteras R.: Engineering of the carbohydrate moiety of fungal glycoproteins to a mammalian type. Symposium From the Gene to the Clinic, Ghent, Belgium, 14-15 November (1997).
16. Schraml J.: <sup>29</sup>Si NMR and its applications in organic chemistry. Encontro-seminario Espectrometria de Ressonancia Magnetica Nuclear, Coimbra, Portugal, 20-21 October (1997).

## Miscellaneous

### International Advisory Board of ICPF

Prof. R. Billet, Ruhr-Universität Bochum, Bochum, FRG  
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Prof. A. Laurent, LSGC-CNRS-ENSIC, Nancy, France  
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Prof. J. Y. Oldshue, Oldshue Technologies Inter. Inc., Fairport, USA  
Prof. R. Pohorecki, Warsaw Technical University, Warsaw, Poland  
Prof. J. J. Ulbrecht, OFI Technology Services, Rockville, USA  
Prof. K. Yoshida, University Tokyo, Tokyo, Japan

### Organization of International Conferences and Scientific Meetings

XIIth FEICHEM Conference on Organometallic Chemistry, Prague, 31st August - 5th September (1997)

Liquid Matter Workshop, Benecko, Czech Republic, 3-5 October 1997

Spring School on Advanced Methods in the Statistical Mechanics of Liquids, 21-25 May, 1997, The Orlik Dam Lake, Czech Republic

### Memberships in Editorial Boards

K. Jeřábek: "Reactive and Functional Polymers"  
T. Boublík: "Fluid Phase Equilibria"  
I. Wichterle: "ELDATA: International Electronic Journal of Physico-Chemical Data"  
R. Ponec: "Advances in Molecular Similarity (JAI Press)"  
K. Klusáček: "Inovační podnikání a transfer technologií"  
J. Drahoš: "International Journal of Multiphase Flow"  
P. Mitschka: "Collection of Czechoslovak Chemical Communications"  
J. Hetflejš: "Collection of Czechoslovak Chemical Communications"  
J. Hetflejš: "Chemické listy"

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