

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 1996

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GENERAL INFORMATION

The Institute of Chemical Process Fundamentals (ICPF) is one of the 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 Ph.D. studies in the field of chemical engineering, physical chemistry, industrial chemistry, and biotechnology.

MANAGEMENT

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

DEPARTMENTS

Department of Diffusion and Separation Processes	(page 5)
E. Hála Laboratory of Thermodynamics	(page 11)
Department of Catalysis and Reaction Engineering	(page 18)
Department of Multiphase Reactors	(page 24)
Department of Biotechnology and Environmental Processes	(page 33)
Department of Reaction Engineering in Gas Phase	(page 38)
Department of Analytical Chemistry	(page 46)

STAFF
(31 December 1996)

Category	Number of Employees
Research	111
Technical	18
Administrative	20
Services	20

BUDGET 1996
(in thousands of Kč; 27 Kč = 1 US\$, approx.)

Institutional support from the National Budget	37 634
Research funds from Grant Agencies	11 046
Contracts with industry	1 887
Total	50 567

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: M. Chačaturjan, L. Hanková, V. Jiříčný, J. Procházka, Z. Prokop, J. Roček,
H. Sovová, P. Uchytíl, E. Volaufová, R. Tomovska
Part time: Z. Brož, V. Staněk, H. Vychodilová
Technical staff: D. Karfík, M. Šoltysová, 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 polymeric 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
- Supercritical fluid extraction; solubilities of liquids in dense CO₂ 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

Polymer-supported ligands for ecological problems

(K. Jeřábek, joint project with The 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 dialkyl dithiophosphoric acid (DADTPA) on porous polymer carriers were investigated [Ref. 8]. Analysis of relations between adsorption of DADTPA from alcoholic solutions and morphology of the polymer supports revealed very unusual mechanism when, instead of a surface adsorption, DADTPA fills the pores gradually from the smallest ones up to those of diameter approx. 10 nm [Ref. 5]. The research was recently expanded to the investigation of supporting of DADTPA on functionalized carriers [Ref. 20].

Ion exchanger catalysts with increased lipophilicity

(K. Jeřábek, joint project with PICT; supported by GA CR, grant No. 104/94/0749)

Catalytic properties were investigated of adsorption-assisted catalysts prepared by partial sulfonation of copolymer of styrene (S) and divinylbenzene (DVB) and by copolymerization of *p*-styrenesulphonyl chloride (SSC) with S and DVB. For reactions in diluted aqueous solutions of organic compounds, a significant positive effect was found of presence of lipophilic unfunctionalized domains in the catalysts [Ref. 14, 34]. For industrially important synthesis of bisphenol A, a method was found how to decrease absorption of water in the ion exchanger catalyst. It may improve the catalyst activity at conditions occurring in the reactor at higher conversion of the reaction mixture. Currently available methods for description of the internal morphology of synthetic resins [Ref. 26] and polymeric networks as catalytic supports were critically reviewed [Refs. 22-25, 30].

Molecular accessibility of microporous matrixes

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

Macromolecular structure and chemical accessibility of swollen polyacrylamide resins were examined with electron spin resonance and inverse steric exclusion chromatography (ISEC). The results in tetrahydrofurane were interpreted on the basis of a physico-mathematical model [Ref. 13]. ISEC-derived description of the working-state morphology of polymer catalysts was confronted with catalytic experiments [Refs. 1, 2].

Quasi-stationary regime in packed column close to the flooding point

(V. Staněk, supported by GA CR, grant No. 104/94/1027)

Transient behaviour of liquid hold up and pressure drop in gas-liquid counter-current packed column was experimentally studied as a response to periodic step changes in gas or liquid flow [Ref. 6]. Experimental data were fitted to mathematical models [Ref. 19] employed in the control theory. The research has also been aimed at constructing physical models of complex multiphase systems [Refs. 38, 39].

Extraction of organic acids by tertiary amines: effect of acid structure and solvent composition

(A. Heyberger, supported by ICPF ASCR)

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. 7, 17, 33]

Development of method and equipment for the determination of persistent organic pollutants in food production chains

(A. Heyberger, joint project with the Institute of Landscape Ecology ASCR; supported by the Ministry of Environment)

A method for quantitative determination of very low concentrations of persistent pollutants (e.g. pesticides and their transformation products) in surface waters was developed. The work included development of an efficient extractor for recovering the pollutants from aqueous samples to suitable organic solvents [Refs. 3, 4, 29, 41, 42].

Supercritical fluid extraction - experiment and modelling

(H. Sovová, participation in the project supported by GA ASCR, grant No. A472413 - see E. Hála Laboratory of Thermodynamics)

Mass transfer model developed at ICPF was applied to extraction of fatty oil with supercritical carbon dioxide [Ref. 9]. The model parameters based on both literature data and our own experiments were mutually compared [Ref. 37]. Measurement of solubilities of three low-volatile liquids in carbon dioxide was finished [Ref. 18], and the research was focused on the solubility of these liquids in carbon dioxide modified by n-heptane, toluene and ethanol [Ref. 36].

International cooperations

University of Padua, Padua, Italy: Molecular accessibility of microporous matrixes

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

Laboratoire des Matériaux Organiques CNRS, Lyon-Solaize, France: Polymer catalysts

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

MIT, Boston, USA: Modelling of cupola furnace

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

Visits abroad

K. Jeřábek: University of Barcelona, Catalan University, Barcelona, Spain; The Weizmann Institute of Science, Rehovot, Israel; Universities of Padua and L'Aquila, Italy

P. Roček: University of Glasgow, Great Britain (11 months)

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

Visitors

M. Boaro: University of Padua, Italy (6 months)

Teaching

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

Publications

Papers

1. Biffis A., Corain B., Cvengrošová Z., Hronec M., Jeřábek K., Králik M.: Relationships between physico-chemical properties and catalytic activity of polymer-supported palladium catalysts. II. Mathematical model. *Appl. Catal. A* 142, 327-346 (1996).
2. Boaro M., Corain B., Lora S., Palma G., Palumbo M., Zecca M., Jeřábek K.: A viable route to designable chiral macromolecular supports: Implications for supported metal catalysis. *J. Mol. Catal. A* 109, L81-L84 (1996).
3. Heyberger A., Tříška J.: Způsob a zařízení pro zakoncentrování málo těkavých organických polutantů z vody pomocí kapalinové extrakce organickými rozpouštědly. (Czech) Method and technology for pre concentration of low volatile pollutants from waste-waters by a batch liquid extraction. *CHEMagazín* 6(3), 16-17 (1996).
4. Heyberger A.: Kolonový reaktor s vibrujícími patry VPE pro extrakce kapalin. (Czech) Vibrating plates extractor for liquid-liquid extraction. *Extraction technology and equipment. CHEMagazín* 6(4), 20-21 (1996).
5. Jeřábek K., Hanková L., Strikowsky A. G., Warshawsky A.: Solvent impregnated resins: Relation between impregnation process and polymer support morphology: I. di-(2-ethylhexyl)dithiophosphoric acid. *React. Funct. Polym.* 28, 201 (1996).
6. Jiříčný V., Staněk V.: An experimental set-up to measure flow transients in a counter-current packed bed column. *Chem. Biochem. Eng. Quart.* 10, 55 (1996).
7. Procházka J., Heyberger A.: Correlation of ternary liquid-liquid equilibria in system isobutyl acetate-acetic acid-water. *Chem. Eng. Sci.* 51, 893-903 (1996).
8. Strikowsky A. G., Jeřábek K., Cortina J. L., Sastre A. M., Warshawsky A.: Solvent impregnated resins (SIR) containing dithiophosphoric acid on Amberlite XAD-2: Extraction of copper and comparison to the liquid-liquid extraction. *React. Polym.* 28, 149 (1996).
9. Šťastová J., Jež J., Bártlová M., Sovová H.: Rate of the vegetable oil extraction with supercritical CO₂. III. Extraction from sea buckthorn. *Chem. Eng. Sci.* 51, 4347-4352 (1996).
10. Uchytíl P., Nguyen Q. T., Clement R., Grosse J. M., Essamri A.: Diffusion of acetic acid and water through poly(vinyl alcohol) membranes. Coupling effects. *Polymer* 37, 93-100 (1996).
11. Uchytíl P.: Pore-size determination in the separation layer of a ceramic membrane using the permeation method. *J. Mater. Sci.* 31, 6293 (1996).
12. Vašák F., Epstein N.: Regression analysis of a chemical reaction fouling model. *Can. J. Chem. Eng.* 74, 173-175 (1996).
13. Zecca M., Biffis A., Palma G., Corvaja C., Lora S., Jeřábek K., Corain B.: Interpenetrating organometallic polymer networks based on poly-dimethylacrylamide-Co-methylene-bisacrylamide: Synthesis and ISEC-ESR characterization. *Macromolecules* 29, 4655-4661 (1996).
14. Jeřábek K., Prokop Z., Revillon A.: Adsorption-assisted catalysts. *React. Funct. Polymers* (in press).
15. Jeřábek K.: Relations between adsorbent morphology and mechanisms of adsorption in solid-liquid systems. NATO ASI Series "Physical adsorption: Experiment, theory and application", (J. Fraissard, Ed.), Kluwer, Dordrecht (in press).

16. Kulov N. N., Muravyov M. Yu., Vašák F.: Hidrodinamika plnochnogo techeniya v naklonnom lotke. (Russ) Hydrodynamics of film flow in inclined channel. Teor. Osn. Khim. Tekhnol. (in press).
17. Procházka J., Heyberger A., Volaufová E.: Amine extraction of hydrocarboxylic acids. Effect of modifiers on citric acid extraction. Ind. Eng. Chem. Res. (in press).
18. Sovová H., Jež J., Chačaturjan M.: Solubility of squalane, dinonyl phthalate and glycerol in supercritical CO₂. Fluid Phase Equil. (in press).
19. Staněk V., Jiříčný V.: Pressure drop overhoot following an onset of gas flow in counter-current beds. Chem. Eng. J. (in press).
20. Strikovskiy 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. (in press).

Review papers

22. Corain B., Zecca M., Jeřábek K.: Synthetic organic matrices in industrial catalysis: scope, synthesis and nanoscopic morphology. In: Materials design for catalytic applications, Bellussi G. (Ed.), pp. 163-179, Societa Chimica Italiana, Milano (1996).
23. Corain B., Jeřábek K.: Macro- and microporous synthetic organic supports in industrial catalysis. Chim. Ind. (Milan) 78, 563-567 (1996).
24. Corain B., Zecca M., Jeřábek K.: Catalysis and polymer networks. Chem. Rev. (in press).
25. Jeřábek K.: Ion exchanger catalysts. Collect. Czech. Chem. Commun. (in press).

Monographs

26. Jeřábek K.: Inverse steric exclusion chromatography as a tool for morphology characterization. In: Strategies in Size-Exclusion Chromatography, ACS Symposium Series 635 (M. Potschka and P. L. Dubin, Eds.), pp. 211-224, Washington, ACS (1996).

Conferences

27. Brož Z.: Inorganic membranes for separation, pervaporation and chemical reactors (review). 12th Int. Congress CHISA '96, Abstr. C5. 1, 1330, Praha, 25-30 Aug. (1996).
28. Jakeš B., Jiříčný V., Strnad R., Korf R., Beljakov O. V.: Determination of the hydrodynamics of counter-current two phase flow through packed column by methods of experimental identification. 12th Int. Congress CHISA '96, Abstr. P9. 51, 843, Praha, 25-30 Aug. (1996).
29. Jeřábek K.: Ion exchanger catalysts. 12th Int. Congress CHISA '96, Symp. on diffusion in zeolites and other microporous materials, Abstr. G8. 1, 1112, Praha, 25-30 Aug. (1996).
30. Jeřábek K., Hanková L., Prokop Z.: Influence of polymer adsorbent morphology on sorption of pesticides from water. 12th Int. Congress CHISA '96, Abstr. P7. 191, 1111, Praha, 25-30 Aug. (1996).
31. Jeřábek K., Hanková L., Prokop Z.: Influence of polymer adsorbent morphology on sorption of pesticides from water. POC '96 - 7th Int. Conference on Polymer Supported Reactions in Organic Chemistry, Wroclaw, Poland, 24-28 June (1996).
32. Jiříčný V., Staněk V.: An experimental study of a packed column at a limit of flooding. 12th Int. Congress CHISA '96, Abstr. C6. 6, 1114, Praha, 25-30 Aug. (1996).
33. Procházka J., Heyberger A., Volaufová E.: Amine extraction of citric acid: effect of modifiers in binary diluents. 12th Int. Congress CHISA '96, Abstr. C1. 3, 125, Praha, 25-30 Aug. (1996).

34. Revillon A., Jeřábek K., Prokop Z.: Adsorption-assisted catalysts with new acid functional resins. POC '96 - 7th Int. Conference on Polymer Supported Reactions in Organic Chemistry, Wroclaw, Poland, 24-28 June (1996).
35. Schneider P., Uchytíl P.: Characterization of porous membranes by liquid expulsion permoporometry. 12th Int. Congress CHISA '96, Abstr. P3. 47, 222, Praha, 25-30 Aug. (1996).
36. Sovová H., Rat V., Chačaturjan M.: Rozpustnost látek v CO₂ s unašečem. (Czech) Solubility of liquids in CO₂ with entrainer. 23. konferencia SSCHI, Zborník s. 291-294, Závažná Poruba, Slovakia, 3-7 June (1996).
37. Sovová H., Bártlová M.: Extraction from plants with supercritical carbon dioxide - experiments and modelling. 12th Int. Congress CHISA '96, Abstr. C3. 3, 853, Praha, 25-30 Aug. (1996).
38. Staněk V., Katz S., Landefeld C., Smiley L.: Applications of the AFS cupola model. 100th AFS Casting Congress and Castexpo, Philadelphia, Penns., USA, April 20-23 (1996).
39. Staněk V., Jiříčný V.: The hydrodynamics of counter-current flow in packed beds undergoing a change of gas on liquid velocity. 12th Int. Congress CHISA '96, Abstr. C6. 5, 1113, Praha, 25-30 Aug. (1996).
40. Strnad R., Jakeš B., Jiříčný V.: Neural networks in an absorption column identification. 12th Int. Congress CHISA '96, Abstr. P9. 59, 1055, Praha, 25-30 Aug. (1996).
41. Tříška J., Heyberger A.: Extraction aided determination of organic contaminant microamounts in water. Int. Technol. Forum Essentia '96, p. 54, Prague, 8-11 January (1996).
42. Tříška J., Vrchotová N., Heyberger A.: Special techniques for the separation of xenobiotics from the environmental water samples. 10th Int. Symposium "Advances and Applications of Chromatography in Industry", Abstract of Papers, LS 9/1, 45-46, Bratislava, Slovakia, 30 June - 4 July (1996).
43. Uchytíl P.: Pore size determination in separation layer of ceramic membrane using permeation method. 12th Int. Congress CHISA '96, Abstr. C5. 2, 221, Praha, 25-30 Aug. (1996).
44. Vachtová J., Procházka J., Heyberger A., Mrnka M., Schrötterová D.: Reprocessing of spent Co-Mo catalysts from petrochemistry. 12th Int. Congress CHISA '96, Abstr. P3. 13, 768, Praha, 25-30 Aug. (1996).

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
Part time: T. Boublík
Technical staff: S. Bernatová, Š. Psutka, J. Wolfová
PhD students: O. Dahmani, P. Kadlec, M. Předota

Fields of research

- Development of experimental techniques for the determination of fluid phase equilibria
- Determination of fluid phase equilibrium data at normal and high pressures
- Measurement of data for supercritical fluid extraction
- Thermodynamic modelling and processing of thermodynamic data
- Molecular simulations on model fluids and fluid mixtures
- Formulation of molecular theories of fluids and derivation of bulk thermodynamic models based on theory
- Application of statistical-mechanical models to real fluids
- Compilation of bibliographic information on vapour-liquid equilibrium data
- Compilation of critically evaluated and correlated data on saturated vapour pressures of pure substances

Applied research

- Determination of vapour-liquid equilibria in systems containing N-alkylacetamides
- Computerized bibliography of vapour-liquid equilibrium data
- Physico-chemical properties of chlorinated C₂₀ - C₂₄ alkanes

Research projects

Molecular theory-based equations of state for real fluids

(K. Aim, supported by GA ASCR, grant No. 472401)

Parameters of the generalized Kihara intermolecular potential (extended by a dipole moment term) have been calculated from the full second-order perturbation theory for lower linear chloroalkanes; promising results were then obtained from test calculations on thermodynamic properties of mixtures of both the type alkane + alkane and alkane + chloroalkane. The method of direct evaluation of vapour-liquid equilibria by molecular dynamics using Gibbs-Duhem integration has been extended to (two-centre Lennard-Jones fluid) mixtures. Effective interaction

site-site potentials have been constructed and successfully applied to model the state behaviour of fluorinated derivatives of methane and ethylene. Equation of state for methanol, based on the primitive association model, has been derived and tested. [Refs. 1, 7-11, 16, 21, 35, 37, 41, 44, 45]

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)

Measurements of vapour-liquid equilibria in binary systems of the type N-methylacetamide + organic solvent were continued. Accurate data on temperature dependences of the vapour pressures of three isomeric dichlorobenzenes, 1,2,4-trichlorobenzene, dimethyl phthalate, neopentanol, 1-hexanol, 1-heptanol, and 1-octanol 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 chlorinated C₂₀ - C₂₄ alkanes. [Refs. 15, 28, 36, 47]

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 primitive models of water, the so-called extended primitive models, has been developed and studied both theoretically and by means of computer simulations. [Refs. 23-25, 32, 42, 48]

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 behavior and global phase diagrams has been developed. [Refs. 12, 13, 22, 23, 26, 43]

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 behavior of systems with an associated component. A new method of the numerical integration of equations of motion of molecular dynamics has been developed. [Refs. 3, 22, 26, 30]

Supercritical fluid extraction - experiment and modelling

(I. Wichterle, supported by GA ASCR, grant No. 472413)

Gas-liquid equilibrium data for the CO₂ + alkyl alkanolate systems were measured at pressures up to 10 MPa at isothermal conditions in the near critical region of CO₂. Solubility of anethole in supercritical CO₂ was determined. Kinetics of supercritical fluid extraction was studied for natural raw materials (peppermint, iris, juniper, etc.). The correlation procedure for fluid phase equilibrium data was completed and applied to the generalization of interaction parameters in equations of state. [Refs. 34, 50, 51, 54, 55; see also Department of Diffusion and Separation Processes, Refs. 9, 18, 36, 37]

Phase equilibria and state behaviour of fluid systems

(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 (naphthene + alkyl alkanoate, pentanols + hexane, systems with aldehydes and N-methylpyrrolidone), ternary, and quaternary systems (C₄ butylchlorides + C₇ hydrocarbons) have been carried out. Data processing: New group (disperse and quasichemical) contributions were evaluated for the DISQUAC and UNIFAC prediction methods. Data base: Vapour-liquid equilibrium data bibliography was supplemented by the end of 1995 and published as a book with a diskette. [Refs. 2, 4-6, 14, 17-19, 33, 40, 52, 53]

International cooperations

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

University of Guelph, Guelph, Canada: Statistical mechanics of fluids

Sonderforschungsbereich, Universität Leipzig, Leipzig, FRG: Simulation of phase and reaction equilibria in inhomogeneous fluids

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

University of Oldenburg, Oldenburg, FRG: High pressure phase equilibria for PSRK (predictive Soave–Redlich–Kwong equation of state)

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 polymer electrolytes

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

Visits abroad

K. Aim: Nihon University, Tokyo; Tokyo Metropolitan University; Hosei University, Tokyo; University of Osaka, Osaka, Japan

O. Drábek: McGill University, Montreal, Canada (12 months)

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

J. Kolafa, I. Nezbeda: University of Guelph, Guelph, Canada (6 months); Rice University, Houston, USA; Texas A&M University, College Station, USA; University of Oklahoma, Norman, USA

J. Linek: ITODYS – Université de Paris, Paris, France

I. Nezbeda: Universität Regensburg, Regensburg; Universität Leipzig, Leipzig, FRG

M. Strnad: Université de Nancy, Nancy, France (6 months)

I. Wichterle: University of Alberta, Edmonton, Canada; University of Illinois, Chicago; University of Delaware, Newark; John Hopkins University, Baltimore, USA

I. Wichterle: Institute of Industrial Chemistry, Warsaw, Poland

Visitors

I. Akiba: Tohoku University, Sendai, Japan (2 months)
A. Dahmani: Université de Science et Technologie, Alger, Algeria (6 months)
Yu. Kalyuzhnyi: Ukrainian Academy of Sciences, Lvov, Ukraine
M. Kettler: Universität Leipzig, Leipzig, FRG
M. Teodorescu: Roumanian Academy of Sciences, Bucharest, Roumania
H. Vörtler: Universität Leipzig, Leipzig, FRG

Teaching

K. Aim: PICT, postgraduate courses “Applied statistical analysis and data processing” and “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: CU, courses “Selected topics in theoretical physics”, “Computer simulation - principles and applications”, and “Applied statistical thermodynamics of fluid systems”

Publications

Papers

1. Aim K., Pavlíček J., Boublík T.: Applicability of the second-order perturbation theory of anisotropic molecule fluids to real systems of constituents differing in molecular size and/or polarity. *Fluid Phase Equilib.* 116, 473-479 (1996).
2. 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).
3. Kolafa J.: Numerical integration of equations of motion with a self-consistent field given by an implicit equation. *Molec. Simulation* 18, 193-212 (1996).
4. Linek J., Wichterle I., Marsh K. N.: Vapor-liquid equilibria for N- methyl-2-pyrrolidone + benzene, + toluene, + heptane, and + methylcyclohexane. *J. Chem. Eng. Data* 41, 1212-1218 (1996).
5. Linek J., Wichterle I., Marsh K. N.: Vapor-liquid equilibria for water + diacetone alcohol, ethyl methanoate + water, and ethyl methanoate + phenol. *J. Chem. Eng. Data* 41, 1219-1222 (1996).
6. Linek J., Wichterle I.: Vapor-liquid equilibria in the hexanal + cyclohexanol and hexanal + cyclohexanone systems at 7.38 kPa. *ELDATA: Int. Electron. J. Phys.-Chem. Data* 2, 19-22 (1996).
7. Lísál M., Vacek V.: Direct evaluation of vapour-liquid equilibria by molecular dynamics using Gibbs-Duhem integration. *Molec. Simulation* 17, 27-39 (1996).
8. Lísál M., Vacek V.: Effective potentials for liquid simulation of the alternative refrigerants HFC-32: CH₂F₂ and HFC-23: CHF₃. *Fluid Phase Equilib.* 118, 61-76 (1996).
9. Lísál M., Vacek V.: Molecular dynamics simulations of fluorinated ethanes. *Mol. Phys.* 87, 167-187 (1996).

10. Lísal M., Watanabe K., Vacek V.: Calculation of second virial coefficients and gaseous viscosities of the refrigerants HFC-32 (CH_2F_2), HFC-23(CHF_3), and HCFC-22(CHClF_2). *Int. J. Thermophys.* 17, 1269-1280 (1996).
11. Lísal M., Vacek V.: Direct evaluation of vapour-liquid equilibria of mixtures by molecular dynamics using Gibbs-Duhem integration. *Molec. Simulation* 18, 75-99 (1996).
12. Nezbeda I., Pavlíček J.: Application of primitive models of association: a simple theoretical equation of state of water. *Fluid Phase Equil.* 116, 530-536 (1996).
13. Nezbeda I., Slovák J.: Can Lennard-Jones particles with bonding sites realistically model water? *Chem. Phys. Lett.* 260, 336-340 (1996).
14. Wichterle I., Linek J.: Isothermal vapor-liquid equilibria in binary mixtures of cyclohexane and methylcyclohexane with n-alkyl (ethyl, propyl, or butyl) ethanoates (acetates) at temperatures from 335 to 370 K. *ELDATA: Int. Electron. J. Phys. Chem. Data* 2, 60-66 (1996).
15. Aim K.: Vapor pressures of 2-chlorotoluene and 4-chlorotoluene and relative volatility in their binary system. *Thermochim. Acta* (in press).
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45. Pavlíček J., Kettler M., Aim K.: State behavior of nonpolar and dipolar fluids of nonspherical molecules from the generalized Kihara model. Liquid Matter Workshop, Strážné v Krkonoších, Czech Republic, 27-29 September (1996).
46. Předota M., Slovák J., Nezbeda I.: Fluid of pseudo-hard bodies. Liquid Matter Workshop, Strážné v Krkonoších, Czech Republic, 27-29 September (1996).

47. Roháč V., Poledníček M., Růžička V., Záborský M., Růžička K., Aim K., Guetachew T.: Vapor pressure and thermal properties of chlorobenzenes under environmental conditions. 12th Int. Congress CHISA '96, Abstr. G5.2, Praha, 25-30 August (1996).
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Part time: D. Arnošt, L. Beránek, K. Klusáček, M. Kraus
PhD students: J. Cinibulk, T. Klicpera, R. Saidur, F. Uhlík

Fields of research

- Catalytic combustion of volatile organic compounds in waste gases
- Dynamics of catalytic systems
- Transport processes in porous solids
- Hydrodechlorination over sulphides
- Sulphide catalysts of unconventional composition
- Unconventional preparation of supported molybdenum catalysts
- Catalytic combustion of methane
- Laser induced oxidative coupling of methane
- 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

Dynamics of multicomponent gas transport in porous solids

(P. Schneider, supported by GA ASCR, grant No. A472408)

Dynamic transport of ternary mixtures in the dynamic version of the Wicke-Kallenbach diffusion cell was studied. It has appeared that the pulse response due to the step change in gas composition could be safely predicted by the mean transport pore model (MTPM) with parameters determined from measurements with binary gases. [Refs. 10, 25-28]

Extra-column effects in the chromatographic technique

(P. Schneider, supported by GA CR, grant No. 104/94/1025)

To determine reliable effective diffusion coefficients of gases in porous solids (catalysts, adsorbents, etc.) from the spreading of the tracer response peaks, it is imperative to take into

account the tracer spreading in the spaces outside the chromatographic column (connecting elements, detector, etc.). The importance of these extra-column effects (ECE) was experimentally demonstrated. A method, based on convolution of the ECE peaks with column response peaks, was developed which permits accurate determination of rate parameters by the chromatographic technique. [Refs. 9, 20, 38, 39]

Experimental verification of dynamic models of catalytic and separation processes

(K. Klusáček, supported by GA CR, grant No. 104/96/0584)

Dynamic models of complex catalytic and separation processes will be experimentally verified and numerical methods for solution of coupled transport-reaction (-adsorption) systems will be further developed. Numerical methods were successfully tested for the prediction of unsteady behaviour of water-gas-shift reaction and adsorption of amines on γ -alumina. The method for estimation of parameters of diffusion model (properties of porous solids) will be developed as well. [Refs. 10, 25, 26]

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.

Preparation of supported molybdena catalysts by unconventional impregnation with molybdic acid

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

The $\text{MoO}_3/\text{Al}_2\text{O}_3$ and MoO_3/C catalysts were prepared by a new clean and simple method of impregnation with molybdic acid. No other chemicals besides MoO_3 and water are used in the impregnation. High loading of 18% $\text{MoO}_3/\text{Al}_2\text{O}_3$ and 31% MoO_3/C were achieved. The activity of sulphided form of the catalysts in hydrodesulphurization of thiophene was the same as of catalysts prepared by conventional impregnation with ammonium molybdate. Catalytic activity measurements and XPS and XRD data indicated the formation of monolayer of MoO_3 over alumina. [Refs. 2, 12]

Hydrodechlorination over unconventional sulphide catalysts

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

Catalytic properties in parallel hydrodechlorination of dichlorobenzene and hydrodesulphurization of methylthiophene of transition metal sulphides supported on active carbon were compared across Periodic Table. Activity and selectivity behaviour was discussed in relation to the disposal of chlorinated organic wastes and to the theory of catalysis over sulphides. [Ref. 11]

Hydrorefining catalysts promoted by noble metals

(Z. Vít, supported by GA CR, grant No. 104/96/0573)

Catalytic properties of Ir as a potential promoter were studied in parallel hydrodesulphurization of thiophene and hydrodenitrogenation of pyridine. Activity of Ir catalysts for N and S removal was much higher than that of the conventional Ni-Mo system. Catalyst efficiency was influenced by the type of the Ir impregnation salt, Ir dispersion and presence of sulphur.

Surface study of the $\text{MoO}_3/\text{Al}_2\text{O}_3$ system

(Z. Vít, supported by GA CR, grant No. 104/96/0573)

Interaction between MoO₃ and OH groups of alumina was studied on a set of catalysts with different MoO₃ loading. The amount of support OH groups consumed per mole of deposited MoO₃ decreased with increased loading in accordance with formation of different surface Mo structures. [Ref. 41]

Catalytic combustion of methane

(K. Jirátová, joint project with PICT; supported by GA CR, grant No. 104/94/1021)

In the combustion of methane, the concentrations of NO_x and CO in the flue gases of a burner have been studied as a function of air excess for various combinations of catalytic components (Pt, Pd, La and perovskites) supported on ceramic foams. [Refs. 14, 33]

Laser induced oxidative coupling of methane

(K. Jirátová, supported by GA CR, grant No. 203/94/1020)

Effect of reaction conditions (amount of catalyst, pulse energy, reaction temperature), active components (perchlorates) and supports on catalyst activity and selectivity was studied. Low reaction temperature of 120°C was sufficient to obtain 80% conversion of methane. The best selectivity to C₂⁺ hydrocarbons was observed at the conversion of methane of 15%. With high pulse energy, acetylene was identified as main reaction product. [Refs. 13, 32, 34]

Chemical applications and theoretical interpretation of pair density matrices

(R. Ponec, supported by GA ASCR, grant No. A4072606/1996)

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. 1, 3, 5, 7, 8, 18, 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 rationalization of structure-(re)activity relationships. [Refs. 4, 6, 15-17, 19]

International cooperations

Theory of chemical reactivity: University of Liverpool, Liverpool, UK, Universität Hannover, Hannover, FRG, University of Buenos Aires, Buenos Aires, Argentina
Catalytic oxidation of VOC and Catalysis over sulphides: Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

Visits abroad

P. Čapek: Institut für Angewandte Chemie, Berlin, FRG (3 months)

K. Jirátová: Royal Institute of Technology, Stockholm and Chalmers University of Technology, Goteborg, Sweden

Z. Vít, National Institute of Materials and Chemical Research, Tsukuba, Ibaraki, Japan (3 months)

Visitors

Y. Sakashita, Advanced Technology and Research Institute, Kanagawa, Japan

H. Katsuno, Idemitsu Kosan Co., Chiba, Japan

A. Spojakina, Institute of Catalysis, Sofia, Bulgaria

G. Eigenberger, University of Stuttgart, FRG

Teaching

K. Jiráťová: PICT, postgraduate course "Preparation of heterogeneous catalysts"

M. Kraus: PICT, postgraduate course "Applied catalysis"

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

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11. 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.* (in press).
12. Hillerová E., Morishige H., Inamura, Zdražil M.: Formation of monolayer of molybdena over alumina by unconventional slurry impregnation or solvent assisted spreading method. *Appl. Catal. A* (in press).
13. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laser induced oxidative coupling of methane. *Catal. Lett.* (in press).
14. Jiráťová K., Morávková L., Malecha J., Koutský B.: Perovskites on ceramic foams as catalysts for combustion of methane. *Collect. Czech. Chem. Commun.* (in press).
15. Ponec R., Yuzhakov G., Pecka J.: Similarity approach to chemical reactivity. Torquoselectivity in pericyclic reactions. *J. Math. Chem.* (in press).
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18. Ponec R., Mayer I.: Investigation of some properties of multicenter bond indices. *J. Phys. Chem.* (in press).
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23. Kraus M.: Dehydrogenation of Alcohols. Chapter 4. 3. 3 in *Handbook of Heterogeneous Catalysis* (Eds. H. Knözinger, J. Weitkamp, J. Ertl), Verlag Chemie, Weinheim (in press).
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26. Čapek P., Hejtmánek V., Šolcová O., Klusáček K., Schneider P.: Dynamics of gas transport in porous media. 12th Int. Congress CHISA '96, Abstr. B9. 3, 260, Praha, 25-30 Aug. (1996).

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31. Jiráťová K., Morávková L., Literová A., Círová A.: Sorption and catalytic properties of Pt and Pd catalysts useful in a combustion of VOC. 12th Int. Congress CHISA '96, Symp. on Environmental and Safety Engineering, Abstr. P5. 23, 130, Praha, 25-30 Aug. (1996).
32. Jiráťová K., Morávková L., Urbanová M., Pola J.: Laserem indukovaná oxidativní dimerizace methanu na C2 uhlovodíky. (Czech) Laser induced oxidative coupling of methane. 23. konf. Slovenskej spoločnosti chemického inžinierstva, Zborník, s. 199-202, Závažná Poruba, Slovakia, 3-7 June (1996).
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34. Jiráťová K., Morávková L., Urbanová M., Vítek J., Pola J.: Laserem indukovaná oxidativní dimerizace methanu. (Czech) Laser-induced oxidative coupling of methane. XXVIII. Symposium o katalýze, Sb. příspěvků P7, ÚFCh JH AV ČR, Praha, 4-5 November (1996).
35. Ponec R.: Molecular basis of structure-reactivity relationships. Similarity approach. 11th MATH/CHEM/COMP Conference, Dubrovnik, Croatia, 24-29 June (1996).
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41. Vít Z., Zdražil M.: Interaction of MoO₃ with OH groups of alumina-quantitative study. XXVIII. symposium o katalýze, Sb. příspěvků P18, ÚFCh JH AV ČR, Praha, 4-5 November (1996).

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J. Tihon, O. Wein, J. Wichterlová, K. Wichterle
Part time: P. Mitschka, J. Vrba
Technical staff: S. Nováková, A. Zemek (part time)

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

- Removal of heavy metals from waste waters

Research projects

Chaotic hydrodynamics of bubble columns

(J. Drahoš, supported by GA CR, grant No.104/95/0647)

The transition from bubbling to jetting regime in nitrogen-water system was studied experimentally by measuring pressure fluctuations in the gas chamber and velocity of liquid circulations near the orifice. The transition from bubbling to jetting regime (transition regime) displayed intermittent character with the hyperbolic distribution of bubbling portion in the pressure signal indicating type III intermittency. The results implied that liquid circulations with $1/f$ noise induced by bubbles affected the bubble dynamics itself as a feed-back and caused the intermittent regime transition. The point of the regime transition was indicated by a sudden drop of Kolmogorov entropy, correlation dimension of the attractor, and Mann-Whitney statistic calculated from pressure signal. An explanation for this drop was suggested on the basis of combination of properties of two attractors coexisting/competing within the intermittency range. [Refs. 18, 29, 40, 41]

Utilization of coal based materials for removal of heavy metals from waste solutions

(J. Drahoš)

Combustion of metal-loaded low rank brown coal was studied in the CFB pilot-plant unit (100 kW). The behavior of metals during the combustion was studied together with their distribution among the bed ash and scrubber sludge. The possibility of metal extraction from the ash by chlorination at high temperatures was also examined. [Refs. 27, 39, 40, 52]

Fuzzy sets as fractal structures

(M. Punčochář)

A new procedure for construction of fuzzy number was developed, based on the covering of points by consequently contracting intervals. The approach leads to the membership function in the form of Devil's staircase, a borderline fractal finding many applications in the modern physics. A method for decomposition of aggregated fuzzy subsets formed by a superposition (generally non-linear) of two fuzzy quantities was proposed. [Refs. 7, 8, 17, 21, 22]

Experimental verification of CFD models in agitated vessels

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

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

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. 23, 24, 44, 45, 46, 47]

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). [Ref. 48]

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. [Refs. 1, 43, 56]

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 and experimentally tested for the wavy flow of viscous liquids along plates with extremely low inclination. [Refs. 48, 50]

Apparent wall slip in microdisperse liquids

(O. Wein, joint project with PICT and the Institute for Hydrodynamics of ASCR; supported by GA CR, grant No. 104/94/1028)

The apparent slip effect has been studied by using the commercial rotational rheometer RheoStress RS100. The device was recalibrated by using an original computer-aided approach (so-called local filtering), and the necessary software was debugged and tested. The system with coaxial disks is proven to be capable of measuring the strong apparent wall slip effect. [Refs. 54, 58]

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 naked golden electrodes. The method was applied to the evaluation of oxygen permeability in new biocompatible materials. [Ref. 62]

Rotational flows of gas-liquid systems

(K. Wichterle, supported by GA CR, grant No. 104/95/0656)

Circulation of bubbles in impeller induced flow and periodic formation of gas cavities at the impeller blades has been studied. New criteria were suggested for modelling the processes in aerated agitated vessels. [Ref. 11]

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. Electrodiffusion measurement has confirmed the validity of the laminar boundary layer theory in the corresponding range of variables and can also be used for investigating the effect of turbulence. The method has been applied in the research of shear rates in centrifugal pumps. [Refs. 9, 12, 20, 23, 24, 43, 44, 47, 49, 57, 63, 64]

Determination of mass transfer capacity of gas-liquid reactors with ejector gas distributors

(J. Zahradník, joint project with PICT; supported by the GA CR, grant No. 104/93/2193)

The effect of ejector configuration on the energy effectiveness of gas-liquid contacting and on the efficiency of gas utilization was examined in the two basic operating modes of ejector-loop reactors, i.e. under conditions of free suction or forced gas supply. Experimental evidence for the free suction regime demonstrated an essential effect of swirl installation on the mechanism of gas-liquid dispersion formation in the ejector and accordingly on the values of gas suction rate and gas holdup in the reactor. Correlation of gas holdup data proved adequacy of the slip velocity concept for the description of gas-liquid flow in ejector loop reactors. [Refs. 16, 26, 32, 67, 68]

Effect of physical properties of the liquid phase on mass transfer capacity of aerated reactors

(J. Zahradník, joint project with PICT; supported by the GA CR, grant No. 104/94/1030).

Experimental programme has been aimed at linking the coalescence characteristics of aqueous solutions of surface active substances (electrolytes, aliphatic alcohols) with hydrodynamic parameters of aerated beds containing such solutions. In addition, an attempt has been made at modifying behaviour of aerated viscous batches by the addition of small amounts of surface active compounds (aliphatic alcohols). [Ref. 37]

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 aimed at examining the effect of design and working parameters on the formation and stability of different bubbling regimes (homogeneous, transition, and heterogeneous) in bubble column and airlift reactors and at identifying the effect of bubbling regime transition on the hydrodynamic and mass transfer characteristics of gas-liquid beds in these reactors. [Refs. 13, 38, 69]

International cooperations

University of Basilicata, Potenza, Italy: Analysis of chaotic time series

University of Rome 'La Sapienza', Italy: Fractals and chaos in hydrodynamics

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

LEMETA, 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: University of Sao Paulo, Sao Paulo, Brazil (1 month); KAIST, Taejon, Korea; University of Tokyo, Tokyo, Japan; University of Rome 'La Sapienza', Rome, Italy

M. Punčochář: Hokkaido University, Sapporo, Japan (3 months); National Central University Chungli, Taiwan

M. Růžička: University of Birmingham, Birmingham, UK; UMIST Manchester, UK

V. Sobolík: LEMETA, INPL, Vandoeuvre les Nancy, France (6 months); University of Munich, Munich, FRG

O. Wein: CNRS UPR 15, Paris, France

K. Wichterle: University of Munich, Munich, FRG

J. Tihon: CNRS UPR 15, Paris, France (9 months)

J. Zahradník: University of Birmingham, Birmingham, UK; UMIST Manchester, UK

Visitors

G. Hetsroni, Technion, Haifa, Israel

K. Yoshida, University of Tokyo, Japan

I. Tsutsumi, University of Tokyo, Japan

T. Usami, NIRE, Tsukuba, Japan

S. K. Sikdar, U.S. EPA, Cincinnati, USA

F. Bishop, U.S. EPA, Cincinnati, USA

C. Hyndman, University of Calgary, Canada

R. Mann, UMIST Manchester, UK

L. L. van Dierendonck, University Twente, Enschede, The Netherlands

H. Haringa, Buss AG, Pratteln, Switzerland

S. D. Vlaev, Institute of Chemical Engineering, Sofia, Bulgaria

A. Ait Ader, University Tizi Ouzou, Algeria

A. Alemany, LEGI/IMG Grenoble, France

F. Binder, LEGI/IMG, Grenoble, France

F. Lusseyran, LEMTA, INPL Vandoeuvre les Nancy, France

B. Izar, LEMTA, INPL Vandoeuvre les Nancy, France

V. Tovchigrechko, ITMO Minsk, Byelorussia (12 months)

Teaching

J. Drahoš: University of Sao Paulo, course "Chaos and Fractals in Chemical Engineering"

J. Drahoš: PICT, course "Fluid Mechanics"

K. Wichterle: TU Ostrava, courses "Process Engineering", "Transport Phenomena", "Reactor Engineering" and "Physical Chemistry of Combustion"

J. Zahradník: PICT, postgraduate course "Multiphase reactors"

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

O. Wein: PICT, course "Chemical Engineering of non-Newtonian Fluids"

Publications

Papers

1. Baleras F., Bouet V., Maurin G., Sobolík V., Tribollet B.: Flow measurement in an impinging jet cell with three-segment microelectrodes. *Experiments in Fluids* 22, 87-93 (1996).
2. Benabes B., Cognet G., Pascal G., Martemyanov S., Sobolík V.: Récentes applications des techniques électrodiffusionnelles en écoulement diphasique. (Fr) Recent applications of electrodiffusion technique in two-phase flow. *La Houille Blanche* 1/2, 129-133 (1996).

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5. Punčochář M., Drahoš J., Vrba J.: Fuzzy number as a product of geometrical construction. *Fuzzy Sets and Systems* 83, 43-49 (1996).
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8. Vrba J., Punčochář M., Drahoš J.: Decomposition of aggregated fuzzy subsets. *SAMS* 22, 255-267 (1996).
9. Wein O.: Generalized transient Léveque problem. *Collect. Czech. Chem. Commun.* 61, 1267-1284 (1996).
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11. Wichterle K., Svěrák T.: Surface aeration threshold in agitated vessels. *Collect. Czech. Chem. Commun.* 61, 681-690 (1996).
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15. Green K. D., Macek T., Zahradník J., Thomas N. H.: Growth parameters of transformed roots. *Biotechnol. Lett.* (in press).
16. Havelka P., Linek V., Sinkule J., Zahradník J., Fialová M.: Effect of the ejector configuration on the gas suction rate and gas holdup in ejector loop reactors. *Chem. Eng. Sci.* (in press).
17. Punčochář M., Drahoš J.: Fractal geometry: a tool for fuzzy reasoning. *J. General Systems* (in press).
18. Růžička M., Drahoš J., Zahradník J., Thomas N. H.: Intermittent transition from bubbling to jetting regime. *Int. J. Multiphase Flow* (in press).
19. Sobolík V., Hoyer K., Bewersdorf H.-W., Gyr A.: Simultaneous wall shear rate measurements by a three-segment electrodiffusion probe and laser-Doppler-anemometry. *Experiments in Fluids* (in press).
20. Sobolík V., Tihon J., Wein O., Wichterle K.: Calibration of electrodiffusion friction probes using voltage-step transient. *J. Appl. Electrochem.* (in press).
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22. Vrba J., Punčochář M., Drahoš J.: Formal uncertainty and membership transfer in fuzzy simulation of complex technological systems. *SAMS* (in press).
23. Wein O., Sobolík V.: Dynamics of electrodiffusion friction probe. I. Shape-dependent potentialstatic transient. *Collect. Czech. Chem. Commun.* (in press).
24. Wein O., Sobolík V., Tihon J.: Dynamics of electrodiffusion friction probes. II. Shape-dependent impedance. *Collect. Czech. Chem. Commun.* (in press).
25. Wichterlová J., Wein O., Kaštánek F.: Particle migration in a Helle-Shaw cell with non-parallel walls. *Int. J. Multiphase Flow* (in press).

26. 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).

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29. 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), World Scientific, Singapore (in press).

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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
- Catalytic dehalogenation of persistent organic pollutants
- 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
- Chiral LC phases - their synthesis and performance

Applied research

- Pilot-scale sorption and biodegradation of PCBs from ground water, performed on an equipment with capacity of 10 m³ per day
- PAH and POP emissions from a leaded and lead-free gasoline-powered engine (in cooperation with OHS Frýdek-Místek and ÚMV-TÚV Praha)

Research projects

Microwave activation of chemical reactions

(M. Hájek, supported by GA CR, grant No. 203/94/1017)

Examination of microwave heating in catalytic reactions proved that heterogeneous reactions were affected by microwaves more efficiently than homogeneous ones. The results indicated that the best reaction conditions were applied in experiments when both activation of catalyst and chemical reactions were carried out under microwave conditions. [Ref. 5]

Chemical degradation of persistent organic pollutants by catalytic dehalogenation on surfaces of inorganic sorbents

(V. Pekárek, supported by GA ASCR, grant No. A4072508)

Dehalogenation experiments have been centered on the substances of the type PCB, PCDD, PCDFs by using inorganic sorbents within the temperature range of 100-350 °C in a closed system. We have dealt here with the opposite process to the novo-synthetic reactions which take place during incineration.

Catalysts for hydrogenation of lipids in cell membranes

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

Ligands for water-tolerant hydrogenation catalysts based on alizarinesulfonate analogs and also on pentamethylcyclopentadiene complexes of Rh(I) were synthesized. Novel Ni(0) and Pd(0) complexes with water-soluble 1,3,5-triaza-7-phosphaadamantane ligand were prepared and their catalytic activity in aqueous systems tested in hydrogenation and oligomerization/telomerization. [Refs. 4, 19]

Study of effect of polychlorinated biphenyls on selected technologically important fungi

(F. Kaštánek, joint project with PICT; supported by the Ministry of Education)

Accumulation of PCBs on selected types of food fungi of the strain *Penicillium* has been studied. Significant adhesion was found for all the sorts of food fungi, which is important with regard to the participation of these pollutants in food chains. Although efficient for PCBs sorption from solutions, fungi do not biodegrade these pollutants (in contrast with, e.g., white rot fungi). Several other techniques of PCBs disposal, including study of bioreactors and biocatalyst immobilization have been reported. [Refs. 15, 29]

Complex method of biodegradation of polychlorinated hydrocarbons (PCBs) in soils and ground water

(G. Kuncová, joint project with PICT, supported by GA CR, grant No. 104/94/1315)

A novel method for bioremediation of soils and ground water contaminated with PCBs and oil pollutants was developed and applied with success in field experiments. [Refs. 7, 14, 20, 22, 23]

Structure of carp gonadotrophin and its bioactivity

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

Special wide porous glass carriers with two different silicon-containing spacers (3-aminopropylsiloxy and 3-(2-aminoethyl)aminopropylsiloxy) were coupled with a biospecific ligand - Concanavalin A - and successfully used in the isolation of gonadotrophin by affinity chromatography. [Ref. 6]

Research and realization of optical fibre sensor for detection of petrol and oil in water and soil

(G. Kuncová, joint project with IRE AS CR, research grant of ČKD Holding OK 259,96)

Monitoring of water pollution with petrols, which are sold in Czech Republic, by optical methods was tested. Three methods were developed for monitoring of contamination in remote places.

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. 13, 17]

Dehalogenation of polychlorinated biphenyls by Fenton's reagent

(J. Včelák, supported by ICPF)

A study of reaction conditions for the oxidative destruction of PCBs in aqueous media by hydrogen peroxide in the presence of Fe(II) salts as catalysts was performed. The applicability of the method was tested on model polychlorinated aromatic hydrocarbons, using the synthetic and analytical experience and instrumentation developed during previous studies of PCBs dechlorination in nonaqueous media. As a part of the above research, dehalogenation of PCBs by means of a complex hydride (sodium dihydridobis(2-methoxyethoxy)aluminate) in nonaqueous media using efficient catalysts - complexes of Co(II) and Ni(II) - was investigated. [Ref. 10]

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

University of Rostock and Max Planck Gesellschaft Arbeitsgruppe Asymmetrische Katalyse, Rostock, FRG: Synthesis of new chiral phases

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

E.N.C.S. de Montpellier, Montpellier, France: Synthesis of new biologically active substances, telomerization

University of Padova, Padova, Italy: Immobilization of enzymes by a sol-gel process

Visits abroad

G. Kuncová: University of Hannover, FRG

G. Kuncová: Cambridge University, UK, course on molecular sensor technology

Visitors

A. Loupy: Université de Paris-Sud, Paris, France

S. Marklund: Umea University, Sweden

Teaching

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

Publications

Papers

1. Čermák Jan, Kvíčalová M., Blechta V., Čapka M., Bastl Z.: Hydrogenation catalytic activity of substituted cyclopentadienyl titanium complexes anchored on polysiloxanes prepared by a sol-gel procedure. *J. Organomet. Chem.* 509, 77-84 (1996).
2. Čermák Jan, Perera S. D., Shaw B. L., Thornton-Pett M.: Pi-2-Methylallylpalladium(II) complexes containing a nine-membered chelate ring with an azine diphosphine ligand: crystal structure of $[(\text{Eta}^3\text{-}2\text{-MeC}_3\text{H}_4)\text{Pd}\{\text{E,Z-PPH}_2\text{CH}_2\text{C}(\text{But})\text{CH}_2\text{PPh}_2\}]\text{Cl}$. *Inorg. Chim. Acta* 244, 115-120 (1996).
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5. Hájek M.: Microwave activation of homogeneous and heterogeneous catalytic reactions. *Collect. Czech. Chem. Commun.* (in press).
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7. Kuncová G.: Lipase immobilized in organic-inorganic matrices. *J. Sol-Gel Sci. Technol.* (in press).
8. 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.* (in press).
9. 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 of the normal-and tangential stresses of ceramic mixture. *SPRECHSAAL - International Ceramics and Glass Magazine* (in press).
10. Včelák J., Hetflejš J.: Catalytic dehalogenation of PCB waste by complex hydrides. *Chemosphere* (in press).
11. Wichterlová J., Wein O., Kaštánek F.: Particle migration in a helle-shaw cell with non-parallel walls. *Int. J. Multiphase Flow* (in press).
12. 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

13. Brányik T., Kuncová G., Páca J., Jurek K.: Biodegradation of phenol by a mixed culture entrapped in SiO₂ films. In: *Progress in Biotechnology 11* (Eds. Wijffles R. H., Buitelaar R. M., Bucke C., Tramper J.), Elsevier, s. 757-761 (1996).
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15. 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* (in press).

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21. Hájek M., Loupy A.: Microwave activation of heterogeneous reactions. XXVIII. Symposium o katalýze, Sb. příspěvků, OP12, Praha, 4-5 November (1996).
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23. Kuncová G., Demnerová K., Burkhard J., Klepaczová I., Chomát M., Matějec V., Berková D., Hüttel I.: Fiber-optic detection of polychlorinated biphenyls. 7th Vienna OPT/R/ODE Workshop, Encl., Regensburg, 17-18 October (1996).
24. Schraml J., Kvíčalová M., Blechta V., Čermák Jan, Herdewijn P.: Tert-butyldimethylsilyl 29Si NMR tag. XIth Int. Symposium on Organosilicon Chemistry, Abstr. PC93, Université Montpellier II, Montpellier, France, 1-6 September (1996).
25. Wichterlová J., Wein O., Kaštánek F.: Particle migration in a Helle-Shaw cell with non-parallel walls. 12th Int. Congress CHISA '96, Symp. on Modelling of dispersed two-phase flow, Abstr. P7. 135, 168, Praha, 25-30 Aug. (1996).
26. Wichterlová J., Wein O., Kaštánek F.: Usazování a drift částice mezi neparalelními stěnami. (Czech) Sedimentation and drift of a particle between non-parallel walls. 23. Konf. SSCHI, Zborník s. 215-218, Závažná Poruba, Slovakia, 3-7 June (1996).
27. Zahradník J., Růžička M., Drahoš J., Kaštánek F., Thomas N. H.: Duality of the gas-liquid flow regimes in bubble column reactors. 12th Int. Congress CHISA '96, Abstr. P5. 105, 63, Praha, 25-30 Aug. (1996).
28. Zikmundová M., Kuncová G., Maléterová Y., Vaněk T.: Utilisation of plant cell cultures for accumulation of metals. 44th Annual Congress of the Society for Medicinal Plant Research and a Joint Meeting with the Czech Biotechnology Society (Ed. I. Valterová), P. 106, Institute of organic chemistry and biochemistry ASCR, Prague, 3-7 September (1996).
29. 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).

Department of Reaction Engineering in Gas Phase

Head: J. Smolík
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Part time: J. Čermák, J. Kocurek
Technical staff: J. Vítek

Fields of research

- Gas-solid reactions
- Gas-solid reactors and operations
- Gas fluidized beds
- Environmental protection
- 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 process
- Particulate emissions from combustion processes
- Transfer processes in dispersed systems
- Nucleation phenomena

Applied research

- Know-how for the combustion of waste organic materials in fluidized bed [Ref. 32]

Research projects

Interrelationships among the main pollutants in the fluidized bed combustion

(M. Hartman, supported by GA CR, grant No. 101/94/0112)

The axial temperature and concentration profiles of methane, oxygen, carbon dioxide and carbon monoxide in an afterburner chamber equipped with a natural gas burner were measured as functions of the throughput and excess air ratio. A simplified model of the unit was developed which includes the two-step combustion kinetics of methane. Aside from carbon monoxide, formaldehyde and acrolein are among the products formed at low temperature and low stoichiometric air ratio. [Refs. 14, 15]

Thermal decomposition of dolomitic hydrated limes

(M. Hartman, supported by GA CR, grant No. 203/94/0111)

The measured data were examined empirically by fitting to the n -th order rate equation of the Arrhenius type, and the kinetic parameters were estimated. A kinetic model has been proposed to correlate the experimental data with the specific surface area of solids. Comparison of the results indicates that particles of magnesium oxide exhibit a surface area which is half an order of magnitude greater than that of calcium oxide sintered under the same conditions. [Ref. 5, 19]

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 analyzed off-line by evaluating their auto-correlations, power spectral density functions and probability density. [Ref. 31]

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_x and N_2O emissions released by combustion in the pressurized fluidized bed have been explored on such factors as operating conditions (temperature, excess air, pressure) and types of functional bonds of nitrogen in the liquid or solid fuel. [Refs. 52-54]

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 products at different temperatures. The studies are to be extended to other olefins. [Refs. 3, 8, 23]

SiC chemical vapour deposition via IR laser induced decomposition of silacyclobutane and 1,3-disilacyclobutane

(J. Pola, joint project with Bergische Universität, Wuppertal; supported by Volkswagen Stiftung FRG)

IR laser induced decomposition of the title compounds was studied at various parameters of laser radiation and found to yield polycarbosilane or α -SiC:H films. The technique is promising for low temperature chemical vapour deposition of SiC-based materials. [Refs. 1, 2, 7]

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. 9, 12, 13]

Deposition of SiO_2 and $\text{Si}_2\text{O}/\text{H}$ 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 for preparation of novel materials containing silicon. SiO_2 and $\text{Si}_2\text{O}/\text{H}$ films from different organosilicon compounds (e.g. disiloxane) are materials with potential applications as semi-conductors. [Ref. 27]

Laser induced sila-derivatization of fullerenes

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

Investigation of reactions of different silacyclobutanes (substituted at silicon with aromatic ring, methyl group and hydrogen) with C_{60} , induced by IR and UV lasers or thermally is a very promising way for preparation of fullerene-containing solid thin films for various applications. [Ref. 6]

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 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. 47, 48, 55]

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 [Ref. 50]. The facility has been also used for study of heterogeneous nucleation of naphthalene vapor on water surface [Ref. 30].

International cooperations

University College London, London, UK: Settling of nonspherical particles

University of Connecticut, Storrs, USA: Reactivity of solids

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

Technical University Cottbus, Germany: Pressurized Fluidized Bed Combustion

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

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

Bergische Universität, Wuppertal, FRG: IR laser chemical vapour deposition of SiC

Sussex University, Brighton, UK: Siladerivatization of fullerenes

The Glasgow University, Glasgow, UK: IR laser degradation of fluoropolymers

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

Visits abroad

J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (1 month)

J. Pola: Bhabha Atomic Research Centre, Bombay, India

J. Pola: Bergische Universität, Wuppertal, FRG (1 month)

J. Pola and M. Urbanová: Sussex University, Brighton, UK (2 weeks)

J. Smolík: University of Helsinki, Helsinki, Finland

J. Smolík: TU Eindhoven, The Netherland

J. Smolík: KIGAM, Taeon, Korea

J. Smolík: National Tsing Hua University, Hsinchu, Taiwan

K. Svoboda: Technical University of Tampere, Tampere, Finland

Visitors

E. A. Volnina: Institute of Petrochemical Synthesis, Moscow, Russia (2 months)

H. Bürger: Bergische Universität, Wuppertal, FRG (1 week)

R. Vatsa: Bhabha Atomic Research Centre, Bombay, India (1 week)

R. Taylor: Sussex University, Brighton, UK (1 week)

S. P. Bakanov: Institute of Physical Chemistry, Moscow, Russia (6 weeks)

M. M. Väkevä: University of Helsinki, Helsinki, Finland (10 weeks)

M. Kulmala: University of Helsinki, Helsinki, Finland (1 week)

Y. Viisanen: Finish Meteorological Institute, Helsinki, Finland (1 week)

A. Laaksonen: University of Helsinki, Helsinki, Finland (2 weeks)

J. Karlsson (IAESTE): Chalmers University of Technology, Göteborg, Sweden (10 weeks)

S. P. Morrin (IAESTE): University of Belfast, Belfast, Ireland (11 weeks)

Publications

Papers

1. Bastl Z., Bürger H., Fajgar R., Pokorná D., Pola J., Senzlober M., Šubrt J., Urbanová M.: Si/C phases from the IR laser induced decomposition of silacyclobutane and 1,3-disilacyclobutane. *Appl. Organometal. Chem.* 10, 83-99 (1996).
2. Dhanya S., Kumar A., Vatsa R. K., Saini R. D., Mittal J. P., Pola J.: Time-resolved study of the transients produced in the CO₂ and ArF laser flash photolysis of gaseous silacyclobutane and 1,3-disilacyclobutane. *J. Chem. Soc., Faraday Trans.* 92, 179-183 (1996).

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4. Hartman M., Trnka O., Vesely V., Svoboda K.: Predicting the rate of thermal decomposition of dolomite. *Chem. Eng. Sci.* 51, 5229-5232 (1996).
5. Jakoubkova M., Bastl Z., Fajgar R., Pola J.: Laser induced chemical vapor deposition of polymeric films from thiophene. *Appl. Surf. Sci.* 106, 67-69 (1996).
6. Pola J., Bastl Z., Šubrt J., Abeysinghe J. R., Taylor R.: Laser induced chemical vapour deposition of Si/C/H materials from monoorganosilanes. *J. Mater. Chem.* 6, 155-160 (1996).
7. Pola J., Ouchi A., Saito K., Ishikawa K., Koga Y.: Efficient chemical vapour deposition of C/H polymeric films by UV laser-induced photolysis of 3-buten-2-one. *Chem. Phys. Lett.* 262, 279 (1996).
8. Samuni U., Fraenkel R., Haas Y., Fajgar R., Pola J.: Environmental effects in the formation of the primary and secondary ozonides of ethylene at cryogenic temperatures. *J. Am. Chem. Soc.* 118, 3687-3693 (1996).
9. Santos M., Diaz L., Bastl Z., Hulinsky V., Urbanova M., Vitek J., Pola J.: IR laser-induced decomposition of 2-chloroethenylsilane for chemical vapour deposition of Si/C phases. *J. Mater. Chem.* 6, 975-981 (1996).
10. Smolik J., Moravec P., Kubat P.: Fine particles synthesis in excimer laser assisted decomposition of tetraethylorthosilicate vapour. *J. Mater. Sci. Lett.* 15, 984-986 (1996).
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12. Urbanova M., Volnina E. A., Guselnikov L. E., Bastl Z., Pola J.: Laser powered homogeneous pyrolysis of 4-silaspiro(3,3)heptane. A source of 2-silaallene and its polymer. *J. Organometal. Chem.* 509, 73-76 (1996).
13. 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 (1996).
14. Vesely V., Hartman M., Trnka O., Fetsch D.: Performance of the afterburner with a natural gas burner. *Fuel* 75, 1271 (1996).
15. Vesely V., Hartman M., Trnka O., Petsch D., Koutsky B., Malecha J.: Účinnost spalování zemního plynu ve fluidní vrstvě. (Czech) Efficiency of the natural gas combustion in a fluidized bed. *Chem. Prům.* 71(7), 23-25 (1996).
16. Ždímal V., Tříska B., Smolik J.: Experiments on thermodiffusiophoresis of droplets in gaseous mixtures. *Colloids Surf. A: Physicochem. Eng. Aspects* 106, 119-125 (1996).
17. Pola J.: Laser-generated organosilicon silenes and their gas-phase polymerization. *Rad. Phys. Chem.* 49, 151 (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 (1997).
19. Hartman M., Trnka O., Beran Z.: Kinetics of the thermal decomposition of hydrated dolomitic lime and sintering of nascent calcine. *Chem. Eng. Commun.* (in press).
20. Hartman M., Beran Z., Vesely V., Svoboda K.: On the transition from homogeneous to bubbling fluidization. *Collect. Czech. Chem. Commun.* (in press).
21. Hartman M., Beran Z., Vesely V., Svoboda K.: Particulate and agregative mode of fluidization. *Chem. Eng. Commun.* (in press).
22. Jirátová K., Morávková L., Urbanova M., Vitek J., Pola J.: Laser induced oxidative coupling of methane. *Catal. Lett.* (in press).

23. Khachatryan L., Fajgar R., Haas Y., Pola J.: Laser-photosensitized homogeneous decomposition of 3,5-dimethyl-1,2,4-trioxolane: the evidence for intermediacy of products of rearrangement. *J. Chem. Soc., Perkin Trans. 2* (in press).
24. Levdansky V. V., Moravec P., Smolík J.: O roste chastits 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).
25. Levdansky V. V., Moravec P., Smolík J.: Zakhvat primesnykh molekul rastushchimi aerazolnymi chastitsami pri lazernom osazhdenii iz gazovoi fazy. (Russ) Trapping impurity molecules by growing aerosols particles in laser deposition from a gas phase. *Vesci Akad. Nauk BR, Ser. Fiz. Khim. Nauk* (in press).
26. Moravec P., Smolík J., Levdansky V. V.: Nano-sized particles from the CO₂ laser assisted decomposition of tetraethylorthosilicate vapour. *J. Matt. Sci. Lett.* (in press).
27. 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.* (in press).
28. Smolík J., Moravec P.: Aerosolové procesy pro přípravu práškových materiálů. (Czech) Aerosol processes for powder synthesis. *Silika* (in press).
29. Smolík J., Moravec P.: Gas phase synthesis of fine silica particles in a tube reactor. *Ceramics* (in press).
30. Smolík J., Schwarz J.: Heterogeneous nucleation of naphthalene vapor on water surface. *J. Colloids Surface* (in press).
31. Trnka O., Hartamn M.: Behaviour of models of chemical g-s reactions in an ideal mixer with gas velocity fluctuations. *AIChE J.* (in press).
32. 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).

Monographs

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34. Punčochář M., Veselý V., Drahoš J., Hayashi J., Chiba T., Tsutsumi A., Yoshida K.: Fluidized bed combustion of coal-based sorbents containing heavy metals. In: *Fluidized Beds & Three-Phase Reactors* (Eds.: W. M. Lu and L. P. Leu), Chin. Inst. Chem. Eng., Taipei, pp. 194-199 (1996).

Thesis

35. Svoboda K.: Vlastnosti a využití vysokoteplotní fluidní vrstvy v metalurgii, při spalování a ochraně ovzduší. Habilitační práce, VŠCHT Praha. (Czech) Properties and application of high temperature fluidized bed processes in metalurgy, coal combustion and air pollution control. Second doctorate, Inst. Chem. Technol., Prague. (1996).

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- 14th Int. Conference on High Resolution Molecular Spectroscopy, Book of Abstracts, p. 260, Prague, 9-13 September (1996).
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58. Ždímal V.: Homogeneous nucleation in supersaturated n-pentanol vapor. Short Course IV. Metastable Behaviour of Fluids and Critical Phenomena, Prague, 30-31 October (1996).

Department of Analytical Chemistry

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Technical staff: J. Lněničková, V. Zimová

Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

Applied research

- Analytical services to research departments of ICPF

Research projects

NMR Spectroscopy of Sterically Demanding Silyl Groups

(J. Schraml, supported by GA CR, grant No 203/94/1026)

A new mechanism of steric effect in ^{29}Si NMR spectroscopy was discovered and quantified. The new effect is due to solvent association which in turn is controlled by solvent accessible surface of the solute. The new mechanism allows interpretation of the many until now unrelated observations which are of considerable significance in analytical applications. [Refs. 7,10]

Materials for Chromatographic Separations of Enantiomers

(M. Bartlová, supported by GA CR, grant No. 104/94/105)

By the reaction of 3-(isocyanatopropyl)triethoxysilane with chiral aminocompounds, the stationary phases have been prepared and then covalently bonded to silica gel. We have concluded that the dependence of capacity factors on volume fraction of the more polar component of mobile phase has been related to the normal phase HPLC system dependence. [Ref. 11]

Steric Effects in MR Spectroscopy

(J. Schraml, supported by GA CR, grant No. 203/96/0567)

The results of the above-mentioned project dealing with steric effects in ^{29}Si NMR are being extended to other fields of NMR to investigate the steric effects in general. [Refs. 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 ^1H , ^{13}C , ^{29}Si and ^{15}N NMR spectroscopy in solution and by X-ray diffraction in the solid state. The aim of the project is to determine the factors responsible for the structure variation. [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 Science: Dynamic NMR

Visits abroad

J. Schraml: Visiting professor at the Catholic University of Leuven, Leuven, Belgium (1 year)

Teaching

J. Schraml: CU, course "NMR Spectroscopy"

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

J. Schraml: Catholic University of Leuven, course "Advanced NMR Spectroscopy"

Publications

Papers

1. Čermák Jan, Kvičalová M., Blechta V., Čapka M., Bastl Z.: Hydrogenation catalytic activity of substituted cyclopentadienyl titanium complexes anchored on polysiloxanes prepared by a sol-gel procedure. *J. Organomet. Chem.* 509, 77-84 (1996).
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4. Van Halbeek H., Schraml J., De Bruyn A., Contreras R., Maras M., Herdewijn P.: Hadamard 1D ^1H tocsy of oligosaccharides. *Glycobiology* 6, 734 (1996).

5. Čermák Jan, Kvičalová 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.* (in press).
6. 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* (in press).
7. Kvičalová 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.* (in press).
8. 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.* (in press).
9. Schraml J., De Bruyn A., Contreras R., Herdewijn P.: A versatile NMR technique for the identification of phosphorylation sites in oligosaccharides. *J. Carbohydr. Chem.* (in press).
10. Van Calenbergh S., De Bruyn A., De Keukeleire D., Herdewijn P., Schraml J., Blaton N. M., Peeters O. M.: Access to a "splitted nucleoside" via a 1,3 dipolar cycloaddition reaction. *J. Chem. Soc., Perkin Trans.* (in press).

Conferences

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12. Čermák Jan, Kvičalová M., Blechta V.: Ni(O) and Pd(O) complexes with triazaphosphaadamantane. Catalysis of butadiene oligomerization/telomerization in an aqueous biphasic system. 10th Int. Symposium on Homogeneous Catalysis, Abstracts p. PP-B54, Princeton, USA, 11-16 August (1996).
13. De Bruyn A., Roose P., Schraml J.: The conformations of alpha, beta-diaminopropionic acid and its beta-oxalyl derivative obtained from 1H-NMR and molecular mechanics calculations. 2nd Int. Conference on the Biology and Toxicity of Lathyrus and Related Genera, King's College London, London, 20 June (1996).
14. De Bruyn A., Maras M., Schraml J., Herdewijn P., Fiers W., Contreras R.: Use of NMR in engineering of the carbohydrate moiety of fungal glycoproteins to a mammalian type. 13th European Experimental NMR Conference, Abstract Book, P. 236, Paris, France, 19-24 May (1996).
15. Schraml J.: From Gemini to Unity (from 200 to 500 MHz) why and when Leuven, Leuven, Belgium, 29 May (1996).
16. Schraml J.: Water suppression. Seminar NMR Spectroscopy, Catholic University of Leuven, Leuven, Belgium, 4 June (1996).
17. Schraml J.: Phase sensitive spectra. Seminar NMR Spectroscopy, Catholic University of Leuven, Leuven, Belgium, 13 June (1996).
18. Schraml J.: NOE in 1D and 2D. Seminar NMR Spectroscopy, Catholic University of Leuven, Leuven, Belgium, 20 June (1996).
19. Schraml J., Kvičalová M., Blechta V., Čermák Jan, Herdewijn P.: Tert-butyldimethylsilyl ²⁹Si NMR tag. XIth Int. Symposium on Organosilicon Chemistry, Abstr. PC93, Université Montpellier II, Montpellier, France, 1-6 September (1996).
20. Sovová H., Bártlová M.: Extraction from plants with supercritical carbon dioxide-experiments and modelling. 12th Int. Congress CHISA '96, Abstr. C3. 3, 853, Praha, 25-30 Aug. (1996).

Miscellaneous

International Advisory Board of ICPF

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Organization of International Conferences and Scientific Meetings

Symposia organized in the framework of 12th International Congress of Chemical and Process Engineering CHISA '96, Praha, 25-30 August 1996:

- Symposium on Modelling of Dispersed Two-Phase Flow
- 2nd Symposium on Dynamics of Catalytic Systems - DCS '96
- Symposium on Diffusion in Zeolites and Other Microporous Materials

Liquid Matter Workshop "Molecular Physics of Liquids: State-of-the-art", Strážné v Krkonoších, Czech Republic, 27-29 September 1996

Memberships in Editorial Boards

K. Jeřábek: "Reactive and Functional Polymers"
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M. Zdražil: "Applied Catalysis A"
K. Klusáček: "Inovační podnikání a transfer technologií"
P. Mitschka: "Collection of Czechoslovak Chemical Communications"
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J. Hetflejš: "Chemické listy"

Notes: