Academy of Sciences of the Czech Republic

Institute of Chemical Process Fundamentals

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ANNUAL REPORT 2001

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GENERAL INFORMATION

The Institute of Chemical Process Fundamentals (ICPF) is one of six institutes constituting the Section of Chemical Sciences of the Academy of Sciences of the Czech Republic. The Institute functions as a center for fundamental research in chemical, biochemical, catalytic and environmental engineering. Besides these activities, the Institute acts as a graduate school for PhD studies in the field of chemical engineering, physical chemistry, industrial chemistry, and biotechnology.

MANAGEMENT

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

DEPARTMENTS

Department of Diffusion and Separation Processes (page 5)
E. Hála Laboratory of Thermodynamics (page 11)
Department of Catalysis and Reaction Engineering (page 17)
Department of Multiphase Reactors (page 24)
Department of Biotechnology and Environmental Processes (page 30)
Department of Reaction Engineering in Gas Phase (page 37)
Department of Analytical Chemistry (page 53)

STAFF

(31 December 2001)

Category	Number of Employees
Research	111
Technical	24
Administrative	16
Services	14

BUDGET 2001

(in million Kč; 38 Kč = 1 US$, approx.)

Institutional support from National Budget	54
Research funds from Grant Agencies	35
Contracts with industry	3

Abbreviations used throughout the Report

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

Department of Diffusion and Separation Processes

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

Fields of research

- Gas capillary condensation in small pores of inorganic membranes and its influence on membrane separation properties
- Relation between the morphology and application properties of polymer catalysts and adsorbents
- Hydrodynamic study of dynamic behaviour of two-phase counter-current gas-liquid flow in packed bed column around flooding
- Amine extraction of sulfuric acid, effect of diluents on extraction equilibrium and third-phase formation; mathematical modelling of Mo(VI) and W(VI) extraction with tertiary amines; determination of organic pollutants in water
- Liquid extraction of drinking and surface waters for determination of toxic pollutants
- Supercritical fluid extraction of natural products; enzymatic reactions in supercritical CO_2; solubilities of liquids and solids in dense CO_2 with entrainer

Applied research

- Extraction aided determination of organic pollutants in waters
- Refining of plant extracts
- Supercritical fluid extraction of biologically active substances from plants
- Preparation of corundum support for ceramic membranes
- Analysis of function of the catalytic reactor for bisphenol A synthesis and research of the catalytic deactivation
- Electrowinning of metals using three-dimensional electrodes

Research projects

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

The possibilities are examined of an increase of catalytic activity of ion exchanger resin catalyst by increasing the degree of their sulfonation beyond the conventional limit of one sulfonic group per monomer unit. It has been found that for proper assessment of the hypersulfonated resin catalysts it is necessary to consider both the influence of the hupersulfonation on the quality of the active centers and the changes in the resin backbone morphology. [Refs. 11, 24]

Study of deactivation of ion exchanger catalysts for synthesis of bisphenol A
(K. Jeřábek, supported by GA ASCR, grant No. S4072002)

Analysis of the behaviour of the industrial reactor for bisphenol A synthesis and laboratory modelling of the catalyst ageing are used for elucidation of the origin of the catalyst deactivation. [Ref. 25]

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

Specific properties of polymers useful as catalyst supports were investigated using combined experimental techniques like inverse steric exclusion chromatography, EPR and NMR. [Refs. 18, 22]

Fundamental research of appearance of pressure and liquid holdup overshoot as a new phenomenon in hydrodynamic behavior of counter-current packed beds
(V. Staněk, supported by GA ASCR, grant No. A4072004)

The pressure and liquid hold up overshoot following sudden increase of gas or liquid flow have been experimentally studied in counter-current packed bed column around flooding point. A mathematical model has been developed to describe the results. [Refs. 3, 9, 28, 29]

Extraction of molybdenum and tungsten by tertiary amines
(A. Heyberger, supported by ICPF)

Results of measurements of sulfuric acid extraction from aqueous solutions with trialkylamine in octanol/kerosene mixtures were correlated. Extraction of tungsten from aqueous solutions of sodium tungstate with solutions of trialkylamine in mixtures of tributyl phosphate in kerosene was investigated. Before the extraction, the organic phase was presaturated with sulfuric acid. Measurements at various values of constant pH were compared. [Refs.4, 23, 30]

Continuous liquid extraction of drinking and surface waters for determination of toxic and ultratrace pollutants
(A. Heyberger, supported by GA CR, grant No. 104/99/1469)

New equipment VPE for determination of organic pollutants was patented. [Ref. 23]

New way of preparing γ- and α-linolenic fatty acids from *Ribes nigrum* seeds: Enzymatic catalysis in supercritical carbon dioxide
(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry and ICT, supported by GA CR, grant No. 203/99/1457)

Enzymatic hydrolysis and ethanolysis of blackcurrant seed oil in supercritical carbon dioxide were performed in a continuous flow reactor. The effect of pressure, temperature, CO_2 flow rate and its moisture on the reactions catalyzed by immobilized lipase Lipozyme

was studied. A survey of potential applications of supercritical fluids as the solvents for enzymatic reactions, particle design, and extraction of biologically active substances as well as in food sterilization was published. [Refs. 7, 20, 27]

Supercritical fluid extraction of plant metabolites usable in the treatment and prevention of the diseases of heart and vessels

(H. Sovová, joint project with Faculty of Pharmacy CU, supported by GA CR, grant No. 203/01/0550)

Lignans from caulomas and leaves of *Schizandra chinensis* were extracted with supercritical CO_2. These substances are of potential use in the food and pharmaceutical industries. The effects of pressure, temperature, modifier concentration, and interaction with vegetable matrix on the course of the extraction process were studied. [Refs. 10, 21]

A potential of nanofiltration layers for membrane separation of light aliphatic hydrocarbons

(P. Uchytil, Joint project with J. Heyrovsky Institute of Physical Chemistry, AS CR, Institute of Physics, AS CR and Institute of Chemical Technology, Prague supported by GA CR, grant No. 104/01/0945)

New sorption and permeation apparatus for the study of surface phenomena during gas transport in Vycor glass pores has been developed and manufactured. The influence of these phenomena on the separation efficiency in Vycor membrane has been experimentally verified. [Ref. 15, 26]

International co-operations

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

Hiroshima University, Hiroshima, Japan: Pervaporation on ceramic membranes

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

Weizmann Institute of Science, Rehovot, Israel: Novel selective sorbents

Technical University, Bratislava, Slovakia: Polymer supported catalysts

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

University of Stellenbosh, Stellenbosh, South Africa: Modelling of back mixing in VPE extractor

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

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

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

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

University of California, Berkeley, USA: Research and development of three-dimensional electrodes for metal electrowinning

Visits abroad

A. Heyberger: University of Durban, AECI, CSIR, Johannesburg, Republic of South Africa (7 weeks)
V. Jiřičný: De Nora, Milan, Italy (4 weeks)

Visitors

S. Boyadzhieva, Institute of Chemical Engineering, Sofia, Bulgaria
B. Corain, University of Padua, Italy
W. Kujawski, Copernicus University, Torun, Poland
I. Mishonov, Institute of Chemical Engineering, Sofia, Bulgaria

Teaching

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

Publications

Original papers

1. Aleksovski S.A., Sovová H., Poposka F.A.: Extraction of Thyme Oil: Comparison between Hydrodistillation and Supercritical CO_2 Extraction. Acta Pharm. 51(4), 305-310 (2001).
2. Corain B., Jeřábek K., Králik M.: Catalysis Inside Synthetic Functional Resins: The Issue of Catalyst Accessibility and Stability. J. Mol. Catal. A Chem. 177(1), 1 (2001).
3. Jiřičný V., Staněk V., Svoboda P., Ondráček J.: Experimental Study of the Flooding and Appearance of a Bubble-Bed on Top of a Counter-Current Packed Bed Column. Ind. Eng. Chem. Res. 40(1), 407-412 (2001).
4. Procházka J., Heyberger A., Horáček J., Volaufová E., Voborská J., Macháčková E.: Extraction of Tungsten with Trialkylamine – Effect of pH. Collect. Czech. Chem. Commun. 66(9), 1407-1419 (2001).
5. Sovová H.: Solubility of Ferulic Acid in Supercritical Carbon Dioxide with Ethanol as Cosolvent. J. Chem. Eng. Data 46(5), 1255-1257 (2001).
6. Sovová H., Stateva P.S., Galushko A.A.: Solubility of ß-Carotene in Supercritical CO_2 and the Effect of Entrainers. J. Supercrit. Fluids 21(3), 195-203 (2001).
7. Sovová H., Stateva R.P., Galushko A.A.: Essential Oils from Seeds: Solubility of Limonene in Supercritical CO_2 and How It Is Affected by Fatty Oil. J. Supercrit. Fluids 20(2), 113-129 (2001).
8. Sovová H., Zarevúcká M., Vacek M., Stránský K.: Solubility of Two Vegetable Oils in Supercritical CO_2. J. Supercrit. Fluids 20(1), 15-28 (2001).

9. Staněk V., Svoboda P., Jiřičný V.: Experimental Observation of Pressure and Holdup Overshoot Following a Sudden Increase of Liquid Flow. Ind. Eng. Chem. Res. 40, 3230-3236 (2001).
10. Bártlová M., Opletal L., Chobot V., Sovová H.: HPLC Analysis of Supercritical Carbon Dioxide Extracts of Schizandra chinensis. J. Chromatogr., B, submitted.
11. Jeřábek K., Hanková L., Prokop Z., Lundquist E.G.: Relations Between Morphology and Catalytic Activity of Ion Exchanger Catalysts for Synthesis of Bisphenol A. Appl. Catal., A, in press.
12. Jiřičný V., Roy A., Evans J.W.: Copper Electrowinning Using Spouted Bed Electrodes. Part 2: Copper Electrowinning with Ferrous Ion Oxidation as the Anodic Reaction. Metall. Mater. Trans. B, submitted.
13. Jiřičný V., Roy A., Evans J.W.: Copper Electrowinning into Spouted Bed Electrode from Conventional Electrolyte. Part 1: DSA Anode for Oxygen Evoluation Used as an Anode. Metall. Mater. Trans. B, submitted.
14. Poposka F.A., Procházka J., Nikolovski K., Tomovska R.: Extraction of Tartaric Acid from Aqueous Solutions with Tri-iso-octylamine (HOSTAREX A 324). Simulation on the Process in a Reciprocating-Plate Extraction Column. Bull. Chem. Technol. Macedonia, submitted.
15. Uchytil P., Petričkovič R.: Vapor Permeation and Pervaporation of Propan-1-ol and Propan-2-ol in Polyethylene Membrane. J. Membr. Sci., submitted.
16. Warshawsky A., Strikowsky A.G., Fernandez F.M., Jeřábek K.: Synthesis of Novel Chelating Resins Containing Dithiophosphoric Functionality and Comparison to Analogous Solvent-Impregnated Resins (SIR's). Sep. Sci. Technol., in press.
17. Warshawsky A., Strikowsky A.G., Vilensky M.Y., Jeřábek K.: Interphase Mobility and Migration of Hydrophobic Organic Metal Extractant Molecules in Solvent Impregnated Resins. Sep. Sci. Technol., in press.

Review papers

18. Corain B., Zecca M., Jeřábek K.: Catalysis and Polymer Network - the Role of Morphology and Molecular Accessibility. J. Mol. Catal. A Chem. 177(1), 3-20 (2001).
19. Kurc L., Veverka P., Petr J.: Výroba peroxidu vodíku přímou syntézou z prvků. (Czech) Production of Hydrogen Peroxide by Direct Synthesis from Elements. Chem. Prum. 72(11), 22-23 (2001).
20. Sovová H., Stateva R.P.: Biologically Active Substances Treated with Supercritical Fluids. Bulgar. Chem. Commun., submitted.

Conferences

21. Bártlová M., Opletal L., Chobot V., Sovová H.: HPLC Analysis of Supercritical CO_2 Extracts of Schizandra chinensis. 2nd International Symposium Separations in the BioSciences SBS 2001, Book of Abstracts, p. 64, Prague, Czech Republic, 17-20 September 2001.
22. Biffis A., Ricoveri R., Králik M., Jeřábek K., Corain B.: Highly Chemoselective Hydrogenation of 2-Ethylanthraquinone to 2-Ethylanthrahydroquinone Catalyzed by Palladium Metal Dispersed Inside Very Lipophilic Functional Resins. XXXIII Symposium on Catalysis, Book of Abstracts, p. 35, Prague, Czech Republic, 05-06 November 2001.
23. Hutton B., Heyberger A., Shabangu S., Miburgh P., Mikus O.: Application of Liquid-Liquid Extraction for Recovery of a Phenolic Antioxidant from an Effluent Stream Using

a Vibrating Plate Extraction Column. 6th World Congress of Chemical Engineering, Book of Abstracts, p. 1406, Melbourne, Australia, 23-27 September 2001.

24. Jeřábek K., Hanková L., Prokop Z.: Hypersulfonated Ion Exchanger Catalysts. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 124, Tatranské Matliare, Slovakia, 21-25 May 2001.
25. Prokop Z., Hanková L., Jeřábek K.: Bisphenol A Synthesis – Modeling of Industrial Reactor and Catalyst Deactivation. XXXIII Symposium on Catalysis, Book of Abstracts, p. 15, Prague, Czech Republic, 05-06 November 2001.
26. Šolcová O., Uchytil P., Petričkovič R., Schneider P.: Pore Size Distribution from Liquid Expulsion Permporometry. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 188, Tatranské Matliare, Slovakia, 21-25 May 2001.
27. Sovová H., Stateva R.P.: Biologically Active Substances Treated with Supercritical Fluids. 9th International Summer School of Chemical Engineering, Proceedings, p. 311, Sozopol, Bulgaria, 18-24 September 2001.
28. Svoboda P., Staněk V., Jiřičný V., Ondráček J.: Experimental Study of Bubble Bed Generated in Counter-Current Packed Bed Column above Flooding Point. 13th International Conference on Process Control 01, Summaries, p. 104, Štrbské Pleso, Slovakia, 11-14 June 2001.
29. Svoboda P., Staněk V., Jiřičný V., Ondráček J.: Liquid Holdup and Pressure Drop Correlation for Counter-Current Packed Bed. (Czech) 13th International Conference on Process Control 01, Summaries, p. 92, Štrbské Pleso, Slovakia, 11-14 June 2001.
30. Volaufová E., Heyberger A., Procházka J., Voborská J.: Extraction of Tungsten and Molybdenum with Trialkylamines. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 126, Tatranské Matliare, Slovakia, 21-25 May 2001.

E. Hála Laboratory of Thermodynamics

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

Fields of research

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

Applied research

- Computerized bibliography of vapour–liquid equilibrium data

Research projects

Phase and state behaviour of fluid systems
(K. Aim, joint project with ICT; supported by GA CR, grant No. 104/99/0136)

Measurements of vapour–liquid equilibria (by dynamic still) have been completed for ternary systems of the types ether + alkanol + hydrocarbon and hydroxyether + alkanol + hydrocarbon and for some of the constituent binaries. A new apparatus for static measurements of high-pressure phase equilibria at elevated temperatures has been tested. Cumulative version of the "Vapour–liquid equilibrium bibliographic database" (on CD-ROM) has been completed and released. [Refs. 1, 2, 31, 32, 48, 49]

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

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

Excess volumes for binary systems of the type octane plus linear 1-chlorohydrocarbon (C_4 to C_6) from 298 to 328 K at normal pressure and for n-heptane + 1-chloropentane and + 1-chlorobutane mixtures at temperatures up to 330 K and pressures up to 400 bar have been measured. The perturbation theory for fluids constituted of anisotropic dipolar molecules has been applied to a series of linear chloroalkanes and further examined by using the newly available data on thermodynamic excess functions for systems of the linear alkane + linear chloroalkane type. [Refs. 5, 7, 20-22, 24-29, 34, 39–41, 44]

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

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

Computer simulations examining in detail the effect of the range of intermolecular interactions on the properties of associating fluids have been extended to mixtures of electrolytes. General rules for developing equations of state from molecular principles have been formulated and a new molecular-based equation of state for water has been derived. [Refs. 4, 9, 12, 13, 30, 33, 43, 45, 47]

Behaviour of liquids at very high pressures: Theory and applications

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

Reaction ensemble Monte Carlo method has been applied to study high temperature plasmas. Molecular mechanisms governing properties of fluids have been examined and general rules formulated. Novel simulation techniques have been developed. [Refs. 3, 8, 10, 11, 13, 19, 32]

High pressure phase equilibria and supercritical extraction

(I. Wichterle, supported by GA ASCR, grant No. A4072102)

Experiments: The high pressure cell for P–V–T measurement (up to 50 MPa, and 670 K) is under construction. The equilibrium cell for vapour–liquid equilibrium determination in systems containing CO_2 was thoroughly renovated. Data processing: Correlation of high pressure gas solubilities using RKS equation of state was elaborated. Supercritical fluid extraction: Modelling of systems with natural raw material (plants).

Statistical–thermodynamic study of model colloid systems

(M. Strnad, joint project with ICT, supported by GA CR, grant No. 203/01/0464)

Molecular simulation codes for model mixtures of hard spheres of considerably different diameters have been developed and various approximations for effective potentials examined.

Molecular thermodynamics of polar and associating fluid mixtures

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

A new molecular-based equation of state for water has been developed. Two-center LJ fluids have been simulated and an improved equation of state developed. [Ref. 13]

International co-operations

DICAMP, University of Trieste, Trieste, Italy: Phase equilibria for supercritical fluid technology
University of Guelph, Guelph, Canada: Molecular based modelling of systems with phase and chemical equilibria; Solubility of organic compounds
Sonderforschungsbereich, University of Leipzig, Leipzig, Germany: Fluids in confined geometries
University of Tennessee, Knoxville, TN, USA: Simulation of complex fluid systems
ITODYS, University of Paris VII, Paris, France: Vapour–liquid equilibrium bibliographic database; Phase equilibria in selected systems
Institute of Physical Chemistry, Romanian Academy, Bucuresti, Romania: Phase equilibria in fluid systems
Northwestern University, Evanston IL, USA: Polarizable models of salt melts
University of Agricultural Sciences, Vienna, Austria: Molecular thermodynamics of polar and associating fluid mixtures

Visits abroad

M. Lísal: North Caroline State University, Raleigh NC, USA (8 months)
I. Nezbeda: University of Tennessee, Knoxville TN, USA (6 months)
M. Předota: University of Tennessee, Knoxville TN, USA (12 months)
J. Slovák: University of Okayama, Japan (2 month)

Visitors

A. A. Chialvo, Oak Ridge National Laboratory, Oak Ridge TN, USA

Teaching

J. Kolafa and I. Nezbeda: CU, course "Introduction to computer simulations in many particle systems"
I. Nezbeda: J. E. Purkyně University, course "Molecular theory of matter"
I. Nezbeda, K. Aim: ICTP, postgraduate course "Applied statistical thermodynamics of fluid systems"

Publications

Original papers

1. Bernatová S., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Ternary System tert-Butyl Methyl Ether + tert-Butanol + 2,2,4-Trimethylpentane and the Three Binary Subsystems. Fluid Phase Equilib. 180, 235-245 (2001).

2. Bernatová S., Wichterle I.: Isothermal Vapour-Liquid Equilibrium in the Binary tert-Butanol or 2,2,4-Trimethylpentane + 1-tert-Butoxy-2-Propanol, and in the Ternary tert-Butanol + 2,2,4-Trimethylpentane + 1-tert-Butoxy-2-Propanol Systems. Fluid Phase Equilib. 189, 111-118 (2001).
3. Kettler M., Vöertler H.L., Nezbeda I., Strnad M.: Coexistence Properties of Higher n-Alkanes Modelled as Kihara Fluids: Gibbs Ensemble Simulations. Fluid Phase Equilib. 181, 83-94 (2001).
4. Kolafa J., Nezbeda I., Lísal M.: Effect of Short- and Long-Range Forces on the Properties of Fluids. III. Dipolar and Quadrupolar Fluids. Mol. Phys. 99(20), 1751-1764 (2001).
5. Kovács É., Aim K., Linek J.: Excess Molar Volumes of (an Alkane + 1-Chloroalkane) at T = 298.15 K. J. Chem. Thermodyn. 33(1), 33-45 (2001).
6. Lee L.C., Kolafa J., Curtiss L.A., Ratner M.A., Shriver D.F.: Molten Salt Electrolytes. I. Experimental and Theoretical Studies of LiI/$AlCl_3$. J. Chem. Phys. 114(22), 9998-10009 (2001).
7. Linek J., Morávková L.: Excess Molar Volumes of the Heptane – 1-Chloropentane System at High Pressures and Elevated Temperatures. Chem. Pap. 55(6), 382-385 (2001).
8. Lísal M., Smith W.R., Nezbeda I.: Accurate Vapour-Liquid Equilibrium Calculations for Complex Systems Using the Reaction Gibbs Ensemble Monte Carlo Simulation Method. Fluid Phase Equilib. 181, 127-146 (2001).
9. Nezbeda I.: Can we Understand (and Model) Aqueous Solutions without any Long Range Electrostatic Interactions. Mol. Phys. 99(19), 1631-1639 (2001).
10. Nezbeda I.: On Molecular-Based Equations of State: Rigor versus Speculations. Fluid Phase Equilib. 182, 3-15 (2001).
11. Nezbeda I.: On Dispersion Force Correction Terms in Perturbed Equations of State. Fluid Phase Equilib. 180, 175-181 (2001).
12. Nezbeda I., Lísal M.: Effect of Short and Long Range Forces on the Thermodynamic Properties of Water. A Simple Short Range Reference System. Mol. Phys. 99(4), 291-300 (2001).
13. Nezbeda I., Weingerl U.: A Molecular-Based Theory for the Thermodynamic Properties of Water. Mol. Phys. 99(18), 1595-1606 (2001).
14. Předota M., Chialvo A.A., Cummings P.T.: On Determination of the Vapor-Liquid Envelope for Polarizable Models by Monte Carlo Simulation. Fluid Phase Equilib. 183-184, 295-300 (2001).
15. Slovák J., Tanaka H., Koga K., Zeng X.C.: Computer Simulation of Water-Ice Transition in Hydrophobic Nanopores. Physica A 292, 87-101 (2001).
16. Smith W.R., Lísal M., Missen R.W.: The Pitzer-Lee-Kesler-Teja (PLKT) Strategy and Its Implementation by Meta-Computing Software. Chem. Eng. Educ. 35(1), 68-73 (2001).
17. Teodorescu M., Aim K., Wichterle I.: Isothermal Vapor-Liquid Equilibrium in the Quaternary Water + 2-Propanol + Acetic Acid + Isopropyl Acetate System with Chemical Reaction. J. Chem. Eng. Data 46(2), 261-266 (2001).
18. Čapla L., Buryan P., Jedelský J., Rottner M., Linek J.: Isothermal P-V-T Measurements on Gas Hydrocarbon Mixtures Using a Vibrating Tube Apparatus. J. Chem. Thermodyn., in press.
19. Kettler M., Nezbeda I., Chialvo A., Cummings P.: Effect of the Range of Interactions on the Properties of Fluids. Phase Equilibria in Pure Carbon Dioxide, Acetone, Methanol, and Water. J. Phys. Chem., submitted.

20. Lísal M., Hall C.K., Gubbins K.E., Panagiotopoulos A.Z.: Self-Assembly of Surfactants in a Supercritical Solvent from Lattice Monte Carlo Simulations. J. Chem. Phys., in press.
21. Lísal M., Hall C.K., Gubbins K.E., Panagiotopoulos A.Z.: Formation of Spherical Micelles in a Supercritical Solvent: Lattice Monte Carlo Simulation and Multicomponent Solution Model. Mol. Simul., in press.
22. Lísal M., Hall C.K., Gubbins K.E., Panagiotopoulos A.Z.: Micellar Behavior in Supercritical Solvent-Surfactant Systems from Lattice Monte Carlo Simulations. Fluid Phase Equilib., in press.
23. Lísal M., Smith W.R., Bureš M., Vacek V., Navrátil J.: REMC Computer Simulation of the Thermodynamic Properties of Argon and Air Plasmas. Mol. Phys., in press.
24. Morávková L., Linek J.: Temperature Dependence of Excess Molar Volumes of (Heptane + 1-Chloroalkane). J. Chem. Thermodyn., in press.
25. Morávková L., Linek J.: Excess Molar Volumes of (Heptane + 1-Chloropentane) at Elevated Temperatures and High Pressures. J. Chem. Thermodyn., in press.
26. Morávková L., Linek J.: Temperature Dependence of Excess Molar Volumes of (Octane + 1-Chloroalkane). J. Chem. Thermodyn., submitted.
27. Morávková L., Linek J.: Excess Molar Volumes of (Heptane + 1-Chlorobutane) at Elevated Temperatures and High Pressures. J. Chem. Thermodyn., submitted.
28. Pavlíček J., Aim K., Boublík T.: Fluids of the Kihara Molecules. II. Binary Mixtures of n-Alkanes. J. Phys. Chem., submitted.
29. Pavlíček J., Aim K., Boublík T.: Fluids of Polar and Polarizable Kihara Molecules. I. Pure Linear Chloroalkanes. J. Phys. Chem., submitted.
30. Předota M., Nezbeda I., Cummings P.T.: Hydrophobic Hydration at the Level of Primitive Models. II. Large Solutes and Water Restructuring. Mol. Phys., in press.

Books and monographs

31. Wichterle I., Linek J., Wagner Z., Kehiaian H.V.: Vapor-Liquid Equilibrium in Mixtures and Solutions. Bibliographic Database. 724pp., ELDATA, Paris 2001.

Conferences

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Department of Catalysis and Reaction Engineering

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Technical staff: H. Součková
PhD students: P. Čuba, J. Rymeš, L. Kaluža

Fields of research

- Catalytic combustion of volatile organic compounds in waste gases
- Transport processes in porous solids
- Sulphide catalysts of unconventional composition
- Unconventional preparation of supported molybdenum catalysts
- Texture of porous solids
- Similarity approach to structure reactivity relationships
- Theoretical analysis of bonding changes and electron correlation in chemical reaction

Applied research

- Catalytic combustion of volatile organic compounds

Research projects

Complex textural characterisation of porous solids regarding the mutual relationship of different methods
(O. Šolcová, supported by GA ASCR, grant No. 4072915)

The standard textural analysis methods (the nitrogen physisorption, mercury porosimetry, helium pycnometry, and liquid-expulsion permporometry) and non-standard transport measurement methods (multicomponent counter-current isobaric diffusion, gas permeation under non-steady state conditions) are applied for complex analysis of pore structure of a broad set of industrial porous solids (monodisperse pore-size distributions, bi- and polydisperse pore-size distributions, with micropores, mesopores and macropores, etc.). The correlation of data obtained from all methods allows a novel approach in determination and prediction of transport parameters characterising processes taking place in porous solids (porous heterogeneous catalysts, membranes, adsorbents, zeolites etc.). [Refs. 3, 19, 24, 27]

Correct characterisation of porous solids for mass transport in pores
(O. Šolcová, supported by GA CR, grant No. 104/01/0546)

The project develops and proves the methods for obtaining material constants of porous solids for description of mass transport in pores (transport parameters) from standard textural analyses (physical adsorption, mercury porozimetry, permporometry). The new counter-current diffusion set-up is designed and constructed. The Graham law is used for description and data evaluation from multicomponent counter-current isobaric diffusion. Verification of the validity of Graham law in porous solids with wide range of pore sizes (from nanometers to tenth and hundredth of micrometers) forms a significant part of the project. [Refs. 14, 41, 42]

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

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

The new "slurry impregnation" method was applied for preparation of supported MoO_3 catalysts. The catalysts were tested in hydrodesulfurization of model compounds and were compared with industrial MoO_3/Al_2O_3 catalysts. High activity MoO_3/MgO catalysts were prepared by the reaction of high surface area MgO with the slurry of MoO_3 in methanol [Refs. 6, 17, 34]. Active carbon supported MoO_3 catalysts were prepared by adsorption of MoO_3 from the slurry MoO_3/water. Very high loadings of about 30% were achieved. It was found that also Co promoter could be deposited by slurry impregnation of MoO_3/C catalyst using CoO. The resulting catalysts were much more active than the corresponding industrial alumina supported samples. [Refs. 4, 32, 33]

Selective Ir-Mo/alumina sulfide catalysts for hydrodenitrogenation

(Z. Vít, supported by GA ASCR, grant No. A4072103)

Mo catalysts modified by small amounts (0.1-0.8 mass %) of highly dispersed Ir were prepared by different procedures and tested in hydrodenitrogenation of pyridine (HDN) and HDS of thiophene. Ir addition has a positive effect on both reactions. A synergy between Ir and Mo was observed in HDN at loading 0.3-0.5 % Ir. Ir interacted with MoS_2 phase and enhanced its reducibility. This is probably related to a greater extent to the formation of anion sulfur vacancies, which are assumed to be active as catalytic sites. A relation between catalysts reducibilities in sulfide and oxide state was discussed [Ref. 17]. The observed effect of Ir was opposite to the effect of conventional Co (Ni) promoters, in contrast to them it was more selective to HDN. [Refs. 44, 45]

Catalytic combustion of volatile organic compounds

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

Catalytic combustion of model organic compounds (toluene, ethanol) was studied with respect to the catalyst composition and the way of its preparation. In preparation of Pt catalysts, effect of platinum particle size and microemulsion composition (various ratio of water, oils and surfactants) on catalytic activity in VOC combustion was examined. Supported salts of phosphomolybdic acids and calcined hydrotalcite-like compounds containing various combinations of transition metal oxides were prepared and characterised from the point of view of their physical chemical properties and catalytic activity in combustion of VOC and methane. [Refs. 9, 15, 20, 23, 28, 29, 39, 40]

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

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

Tungsten heteropolyacid and its Cr, Mn, Fe, Co, and Ni salts supported on alumina have been used to model hydrodesulfurization catalysts of different activity. Promoting effect of countercation on thiophene hydrodesulfurization was studied. The highest activity of Ni

countercation is probably connected with formation of mixed NiOAlW phase. Catalytic activities in hydrodesulphurization (HDS) of thiophene over molybdenum containing catalysts prepared with hexagonal mesoporous silicas were higher than the activity of the catalyst prepared with amorphous silica. Nickel introduced as counter-cation of Keggin structure of heteropoly anion enhanced and stabilised the HDS activity. [Refs. 7, 8, 16, 26, 35, 43]

Sulfide hydrotreating catalysts with unconventional supports
(M. Zdražil, supported by GA CR, grant No. 104/01/0544)

Highly active CoMo and NiMo sulfide hydrodesulfurization catalysts supported over MgO were prepared by new method of non-aqueous impregnation. Texture of high surface area MgO support is unstable in aqueous solutions and the catalysts prepared by conventional aqueous impregnation exhibit low activity. However, MgO support is stable in methanol and the use of this solvent for impregnation provides catalysts that are more stable than the corresponding conventional alumina supported catalysts. [Ref. 22]

Role of electron pairing in chemical bonds
(R. Ponec, supported by GA ASCR, grant No. A4072006)

The project deals with the theory of chemical bond, especially in the evaluation of the role of electron pairing in chemical bonding. For this purpose, a new procedure, based on the analysis of the so-called domain averaged Fermi hole, was recently proposed. The approach was applied to the elucidation of bonding in several molecules containing complex bonding patterns like the multicenter bonds, hypervalence, etc. [Refs. 2, 5, 10-12]

Design of theoretical QSAR models based on quantum similarity data
(R. Ponec, supported by grant Ministry of Education, D0.20)

The project deals with the theoretical approach to the design of new structure-activity relationships based on the systematic use of similarity measures and indices as new theoretical descriptors. The project is solved in the collaboration with the Institute of Computation Chemistry of the University of Girona. [Ref. 1]

International co-operations

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

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

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

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

Visits abroad

T. Klicpera: University of Tokyo (12 months)

Visitors

D.L. Cooper, University of Liverpool, UK
L. Line, University of Pais Vasco, Bilbao, Spain
D. Klvana, École Polytechnique, Montreal, Canada (4 months)
J. Kirchnerová, École Polytechnique, Montreal, Canada (4 months)

Teaching

K. Jirátová: ICT, postgraduate course "Preparation of heterogeneous catalysts"
R. Ponec: CU, course "Reaction mechanisms in organic chemistry"
P. Schneider: ICT, postgraduate course "Texture of porous solids"
M. Zdražil: ICT, postgraduate course "Preparation of heterogeneous catalysts"

Publications

Original papers

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14. Šolcová O., Šnajdaufová H., Schneider P.: Multicomponent Counter-Current Gas Diffusion in Porous Solids: The Graham's-Law Diffusion Cell. Chem. Eng. Sci. 56, 5231-5237 (2001).
15. Spojakina A.A., Kostova N.G., Sow B., Stamenova M., Jirátová K.: Thiophene Conversion and Ethanol Oxidation on SiO_2-Supported 12-PMoV-Mixed Heteropoly Compounds. Catal. Today 65(2-4), 315-321 (2001).
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29. Jirátová K., Čuba P., Kovanda F., Hilaire L., Pitchon V.: Preparation and Characterisation of Hydrotalcites Ni-Mg-Al for Combustion Catalysis. 5th European Congress on Catalysis EuropaCat V, Abstracts, p. 1-0-12, Limerick, Ireland, 02-07 September 2001.
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45. Vít Z., Zdražil M., Cinibulk J.: Comparison of the Effects of Classical Ni(Co) Promoters and Iridium in Model Hydrotreating Reactions over the Mo Catalyst. (Czech). XXXIII Symposium on Catalysis, Book of Abstracts, p. 59, Prague, Czech Republic, 05-06 November 2001.

Department of Multiphase Reactors

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

Fields of research

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

Research projects

Instability of homogeneous flow regime in bubble columns
(M. Růžička, supported by GA CR, grant No. 104/01/0547)

Studies on homogeneous-heterogeneous flow regime transition in gas-liquid bubble columns. Identification of the hydrodynamic mechanism responsible for the instability of the homogeneous flow regime. Investigation of the instability character. [Refs. 1, 9, 10, 20-27]

Increasing the transport coefficients of convective processes by means of jet flow modulation
(V. Sobolík, joint project with CTU, Faculty of Mechanical Engineering, Prague; supported by GA CR, grant No. 101/99/0060)

Convective heat and mass transfer between the fluid jet and the wall placed opposite the impinging jet have been investigated experimentally with the aim to achieve the increase in the value of transfer coefficient by means of applying a periodic modulation of the flow from the nozzle of supply. [Refs. 31-33]

Electrochemical sensors for flow measurements
(V. Sobolík, COST project supported by the Ministry of Education, OC F2.10/1996)

Electrochemical technique for the near-wall flow diagnostics has been improved (sensors manufacturing, development of the control electronics, dynamic response of the sensors). The directionally sensitive segment probes have been applied to study different flow situations (near-wall turbulence, backward-facing step flow, Taylor-Couette flow, impinging fluid jet, wavy film flow). [Refs. 3, 6, 11, 13, 16, 28, 29]

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

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

The stability of the Newtonian film flowing down an oscillating wall has been studied with the aim to predict the effect of parallel wall oscillations on the flow character in the liquid film. The linear stability analysis has provided the criterion for wave inception and the estimation of wave growth rates for different oscillation regimes (film flow stabilization or destabilization). The following experiments (film thickness and wall shear stress measurements) have covered a wide range of the operation parameters: flow rate, inclination angle, liquid properties, and parameters of oscillations. [Refs. 28, 29]

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

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

Experiments on the effect of liquid viscosity and plasticity on gas holdup and stability of homogeneous bubbling regime in bubble column were made. Results for gas hold-up and mass transfer coefficient (k_La) have been obtained for an ejector-loop reactor. Residence time distribution of gas phase in bubble column has been measured and synergy between systems properties and gas dispersion modes examined. An up-to-date literature rewiew of publications concerning the gas holdup and volumetric mass transfer coeficients in bubble type column reactors was prepared. [Refs. 5, 17-19]

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

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

Studies on (i) basic experimental and theoretical hydrodynamics of two-phase bubble beds including effects of viscosity, surface tension, and presence of third phase, (ii) oxygen transfer in bubble-beds, (iii) hydrodynamics of real fermentors as used in food-industry, (iv) CFD simulation of model and real multiphase flows, (v) modelling and improving real reacting systems. [Refs. 1, 9, 10, 20-27, 34-37]

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

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

The project gives young researchers pursuing doctoral studies the opportunity to receive training within diagnostics of multiphase flows. Four PhD students stayed in our laboratory during this academic year.

Rheometric and electrodiffusion study of the apparent wall slip in lyophylic dispersions

(O. Wein, supported by GA CR, grant No.104/01/0545)

Apparent wall slip in several water-soluble polysaccharides was studied experimentally, using rotational viscometry. An extensive collection of the related material functions has been obtained. Viscometric theory was developed for a novel rotational viscometer with coaxial Morse cones. [Ref. 30]

International co-operations

University of Tokyo, Tokyo, Japan: Chaotic hydrodynamics of bubble columns
Aston University, Birmingham, UK: Multiphase chemical reactors and bioreactors
UMIST, Manchester, UK: Gas-liquid reactors for complex rheology fluids
University of Minho, Braga, Portugal: Multiphase bubble bed reactors
CNRS UPR 15, Paris, France: Electrodiffusion diagnostics of flow
CRTT, Saint Nazaire, France: Backward-facing step flows
LEGI / IMG, Grenoble, France: Impinging jets
University of Poitiers, France: Electrochemical sensors for flow measurements
Inst.Chem.Eng., BAS, Sofia, Bulgaria: Gas-liquid reactors for complex rheology fluids
Swiss Federal Institute of Technology, Lausanne, Switzerland: Hydrodynamics of bubbly flow
Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow
University of Thessaly, Volos, Greece: Liquid film flows

Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)
J. Vejražka: LEGI / IMG, Grenoble, France (6 months)

Visitors

L. Gastin-Viennot, École des Mines D'Albi, France (3 months)
D. Bröder, Martin Luther Universität, Halle, Germany (2 months)
V. Höller, Swiss Federal Institute of Technology, Lausanne, Switzerland (3 months)
P. Mena, University of Porto, Portugal (3 months)
M. Sommerfeld, Martin Luther Universität, Halle, Germany
J. C. Sartoreli, A. Tufaile, Univ. Sao Paulo, Brazil

Teaching

J. Drahoš: ICT, course "Fluid Mechanics" and postgraduate course "Multiphase reactors"
M. Fialová: ICT, postgraduate course "Multiphase reactors"
J. Tihon: ICT, postgraduate course "Drops, bubbles and particles"
O. Wein: TU Brno, course "Principles of Rheology"

Publications

Original papers

1. Růžička M., Drahoš J., Fialová M., Thomas N.H.: Effect of Bubble Column Dimensions on Flow Regime Transitions. Chem. Eng. Sci. 56(21-22), 6117-6124 (2001).

2. Růžička M., Zahradník J., Drahoš J., Thomas N.H.: Homogeneous-Heterogeneous Regime Transition in Bubble Columuns. Chem. Eng. Sci. 56(15), 4609-4626 (2001).
3. Tihon J., Legrand J., Legentilhomme P.: Near-Wall Investigation of Backward-Facing Step Flows. Exp. Fluids 31, 484-493 (2001).
4. Vrba J.: Fuzzy Modelling and Simulation - The Evaluating Scales Problem. SAMS 41, 257-288 (2001).
5. Zahradník J., Mann R., Fialová M., Vlaev D., Vlaev S.D., Lossev V., Seichter P.: A Networks-of-Zones Analysis of Mixing and Mass Transfer in Three Industrial Bioreactors. Chem. Eng. Sci. 56(2), 485-492 (2001).
6. Dumont E., Fayolle F., Sobolík V., Legrand J.: Wall Shear Rate in the Taylor-Couette-Poiseuille Flow at Low Axial Reynolds Number. Int. J. Heat Mass Transfer 45, 679-689 (2002).
7. Sobolík V., Žitný R., Tovčigrečko V., Delgado M., Allaf K.: Viscosity and Electrical Conductivity of Concentrated Solutions of Soluble Coffee. J. Food Eng. 51, 93-98 (2002).
8. Drahoš J., Punčochář M.: Comments on Application of the Fractional Brownian Motion in an Airlift Reactor. Chem. Eng. Sci., in press.
9. Růžička M., Drahoš J.: Effect of Viscosity on Homogeneous-Heterogeneous Regime Transition in Bubble Columns. Chem. Eng. Sci., submitted.
10. Růžička M., Thomas N.H.: Convective Instability of a Uniform Horizontal Bubbly Layer Confined by Vertical Walls. Int. J. Multiphase Flow, submitted.
11. Tihon J.: Electrodiffusion Diagnostics of the Near-Wall Flows. Chem. Pap., in press.

Chapters in books

12. Drahoš J., Punčochář M.: Fraktály a chaos: Věda o běžných věcech. (Czech) Fractals and Chaos: Science about Common Matters. In: Vybraná témata na přelomu tisíciletí. (Mareš, M., Nekola, J., Řeřicha, R., Eds.), pp. 33-45, Česká asociace Římského klubu, Praha 2001.

Theses

13. Sobolík V.: Mapování smykových rychlostí v kapalinách. (Czech) Mapping of Shear Rates in Liquids. DrSc. Thesis, Ústav chemických procesů AV ČR, 42 pp., Praha 2001.

Patents

14. Hájek M., Drahoš J.: Způsob a zařízení k tepelnému zpracování přírodních materiálů, zvláště vulkanického původu. (Czech) Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Vulcanic Origin. Czech. Pat. PV 2000-1935 (in press).
15. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Vulcanic Origin. PCTI/CZ00/00042/ (in press).

International conferences

16. Drahoš J.: New Trends in Signal Treatment. 1st Conference "Electrochemical Sensors for Flow Diagnostics", Proceedings, pp. 12-13, Florence, Italy, 07-09 November 2001.

17. Elgozali A., Fialová M., Linek V., Wein O., Zahradník J.: Characteristics of (g)-(1) Contactors with Ejector-Type Gas Distributors for Aqueous Polymer Solutions. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 74, Tatranské Matliare, Slovakia, 21-25 May 2001.
18. Fialová M.: Gas Holdup in Viscous Aerated Solutions. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 144, Tatranské Matliare, Slovakia, 21-25 May 2001.
19. Fialová M.: Gas Holdup in a Bubble Column Reactor Containing Viscous Solutions. 9th International Summer School of Chemical Engineering, Proceedings, p. 190, Sozopol, Bulgaria, 18-24 September 2001.
20. Růžička M., Drahoš J., Fialová M., Thomas N.H.: Correlations for Critical Gas Holdup in Bubble Columns of Different Size. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 145, Tatranské Matliare, Slovakia, 21-25 May 2001.
21. Růžička M., Drahoš J., Fialová M., Thomas N.H.: Effect of Bubble Column Dimensions on Flow Regime Transition. 5th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Conference Papers, Melbourne, Australia, 23-27 September 2001.
22. Růžička M., Drahoš J., Thomas N.H.: Hydrodynamic Interactions in a Bubble Array. EUROMEC 421 Colloquium. Strongly Coupled Dispersed Two-Phase Flows, Book of Abstracts/Resumes, Grenoble, France, 10-12 September 2001.
23. Růžička M., Drahoš J., Thomas N.H.: Effect of Bubble Column Dimensions on Flow Regime Transition. 3rd European Congress of Chemical Engineering, Book of Abstracts [in Chem.-Ing.-Tech. 73(6), p. 535 (2001)], Nuremberg, Germany, 26-28 June 2001.
24. Růžička M., Drahoš J., Thomas N.H.: Dynamic Behavior of a Bubble Chain. 4th International Conference on Multiphase Flow, Book of Abstracts, pp. 88-89, New Orleans, Louisiana, USA, 27 May - 01 June 2001.
25. Růžička M., Smolková P., Wichterle K., Drahoš J.: Effect of Viscosity and Surfactants on Flow Regime Transition in Bubble Columns. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 146, Tatranské Matliare, Slovakia, 21-25 May 2001.
26. Růžička M., Thomas N.H., Drahoš J.: Convective Instability of Uniform Dispersed Layers. EUROMECH 421 Colloquium. Strongly Coupled Dispersed Two-Phase Flows, Book of Abstracts/Resumes, Grenoble, France, 10-12 September 2001.
27. Růžička M., Thomas N.H., Drahoš J.: Convective Instability of Bubbly Layers. 4th International Conference on Multiphase Flow, Book of Abstracts, pp. 95-96, New Orleans, Louisiana, USA, 27 May - 01 June 2001.
28. Tihon J.: Electrodiffusion Diagnostics of the Near-Wall Flows. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 78, Tatranské Matliare, Slovakia, 21-25 May 2001.
29. Tihon J.: Dynamic Response of the Electrodiffusion Friction Probes to Strong Flow Fluctuations in the Near-Wall Region. 1st Conference "Electrochemical Sensors for Flow Diagnostics", Proceedings, p. 16, Florence, Italy, 07-09 November 2001.
30. Večeř M., Wein O.: Polymer Viscometry under Apparent Wall Slip. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 147, Tatranské Matliare, Slovakia, 21-25 May 2001.
31. Vejražka J, Marty P., Sobolík V.: Heat Transfer Experiments in a Submerged Impinging Round Jet Using Liquid Crystal Thermometry. 5th World Conference on Experimental Heat Transfer, Fluid Mechanics, and Thermodynamics 2001, Proceedings, pp. 981-986, Thessaloniki, Greece, 24-28 September 2001.

32. Vejražka J., Marty P., Sobolík V.: Mesure de transfert de chaleur par cristaux liquides:application au jet impactant. (Fr) Heat Transfer Measurements by Liquid Crystals: Application to Impinging Jets. Congres Francais de Thermique, SFT 2001, pp. 167-172, Nantes, France, 29-31 May 2001.
33. Vejražka J., Marty P., Sobolík V.: Une nouvelle méthode de mesure de température par cristaux liquides appliquée aux jets impactants. (Fr) The New Method of Measurement of Temperature Fields Applied to Impinging Jets. Transferts de Chaleur et de Masse Dans Les Jets, Book of Abstracts, pp. 1-8, Paris, France, 14 March 2001.
34. Zahradník J., Růžička M., Markoš J., Teixeira J., Generalis S., Thomas N.H.: Modelling Design of Multiphase Bubble-Bed Reactors for Advanced Food-Industry Applications. 5th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Conference Papers, Melbourne, Australia, 23-27 September 2001.
35. Zahradník J., Růžička M., Markoš J., Teixeira J., Generalis S., Thomas N.H.: Modelling Design of Multiphase Bubble-Red Reactors for Advanced Food-Industry Applications. 3rd European Congress of Chemical Engineering, Book of Abstracts [in Chem.-Ing.-Tech. 73(6), p. 357 (2001)], Nuremberg, Germany, 26-28 June 2001.
36. Zahradník J., Růžička M., Markoš J., Teixeira J., Generalis S., Thomas N.H.: Modelling Design of Multiphase Bubble-Bed for Advanced Food-Industry Technologies. 10th European Congress on Biotechnology, Book of Abstracts, p. 194, Madrid, Spain, 08-11 July 2001.
37. Zahradník J., Thomas N.H., Růžička M., Teixeira J., Markoš J., Generalis S.: Modelling Design of Multiphase Bubble-Red Reactors for Advanced Food-Industry Technologies. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 138, Tatranské Matliare, Slovakia, 21-25 May 2001.

Department of Biotechnology and Environmental Processes

Head: J. Čermák
Deputy: M. Hájek
Research staff: T. Brányik, V. Církva, M. Czakóová, V. Gruber, J. Hájek, J. Hetflejš, F. Kaštánek, D. Klier, G. Kuncová, Y. Maléterová, S. Šabata, J. Včelák
Part time: O. Podrazký
Technical staff: K. Auerová, J. Brustman, J. Kubešová, Z. Soukup, J. Storch
PhD students: I. Jurčová, J. Kurfürstová, M. Pošta, L. Šťastná

Fields of research

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

Applied research

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

Research projects

Revaluation of dangerous waste on the basis of ferric oxides with portion of heavy metals (furnace steel dusts) as a new additive to building materials
(F. Kaštánek, project supported by GA CR, grant No.104/99/0440)

Reserch was focused on the study of materials prepared from cements and additives in cooperation with ICT Prague. Properties of mixtures of Portland cements and "waste steel foundry dust" (WSFD) from steel works were examined. It was found that WSFDs are formed by microporous clusters of spherical particles of iron oxides. The content of ZnO in WSFD affects markedly the hydratation of cement + WSFD mixtures both in solidification time and

strenght development. Cement and WSDF mixtures show long-term strength stability and low heavy metals leaching even at WSFD content of 70-80 mass %. A special attention has been paid to the pastes, i.e. aqueous suspensions of cements with WSFD additives. The properties of mortars and concretes were studied. The perspectives of WSFD solidification, disposal and the use of this waste material as a new additive to building materials were outlined. [Refs. 19, 44]

Biodegradation of phenols in water and water sediments
(F. Kaštánek, supported by GA CR, grant No.104/00/0575)

The aim of this project is to study the biodegradation of phenol adsorbed on real (or artificially contaminated) sediments. The efficiency of biodegradation realized by aerobic oxidation using bacteria strains depends on the size and type of sediment particles and the type of contamination (phenol or mixture of phenol, BTX and PAU). Evaluation of laboratory results led to the proposal of bioreactor configuration in a semi-pilot scale and to the study of the influence of external conditions on the rate of biodegradation.

Novel techniques for implementation of immobilized biocatalysts in industrial processes
(G. Kuncová, supported by INCO-COPERNICUS project Erbic15CT98, and Ministry of Education of the Czech Republic)

The main objective of this project, which started in October 1998, is to facilitate the implementation of new materials and techniques into industrial biocatalytic processes. The project is a concerted action involving multidisciplinary, trans-national teams, to integrate the expertise on immobilized biocatalysts. [Refs. 13, 14, 16, 36]

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

Among the most important results of systematic research of immobilization of biomaterials has been an increasing activity of lipase by entrapement into organic-inorganic matrices. We reported the reproducible and easily scaled-up procedure of a preparation of the biocatalyst which is highly active in organic solvents swelling the silicone polymer matrix. The biocatalyst can be used as flexible sheets several mm thick without decreasing its activity as compared to granulated material. The two-step process was based on immobilization by sorption of enzyme on fine inorganic particles and threir subsequent entrapment into a silicone based polymer. [Refs. 13, 14, 37]

Microwave activation of heterogeneous catalytic reactions
(M. Hájek, supported by ICPF)

Research has been focused on microwave activation of heterogeneous catalytic reactions in liquid phase at low temperature (0 to –176 ^{o}C). It was found on model reaction of transformation of t-butylphenols that microwaves have a strong effect on reaction rate. The results were explained on the basis of superheating. [Refs. 38-40]

Microwave technology of glass melting
(M. Hájek, supported by GA ASCR, grant No. S4072003)

In applied research, a new technology for melting and manufacture of glass by microwave energy has been extended. [Refs. 21, 24, 30, 31]

Microwave activation of photochemical reactions
(V. Církva, suported by ICPF)

Reactions under simultaneous MW and UV irradiation have been studied. [Refs. 12, 20, 28]

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

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

Modification of liquid polybutadienes by organosiloxanes has been studied and testing of their applicability as surface hydrophobic-hydrophilic modifiers started. The results of the study of the kinetics and mechanism of homogeneously catalyzed hydrogenation of OH-telechelic, medium vinyl polybutadienes have been reported. [Ref. 18]

Transition metal complexes with cyclopentadienyl ligands for catalysis in fluorous biphase systems

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

New synthons, 2-(perfluoroalkyl)ethyl triflates, were synthesized and used for the preparation of bis[(perfluoroalkyl)ethyl]cyclopentadienes with various combinations of chain lengths. Partition coefficients of novel perfluoroalkyl-substituted ferrocenes prepared from them in a complex mixture of regioisomers were determined. The catalytic activity of previously prepared (perfluoroalkyl)tetramethylcyclopentadienyl rhodium complexes in supercritical carbon dioxide was studied. [Refs. 1, 2, 7, 15, 25, 26]

New highly active catalysts for the Heck reaction

(J. Čermák, joint project with CU, supported by GA CR, grant No. 203/01/0554)

Rigid pincer palladium complexes containing ene-hydrazone coordinated diphosphino-azines with metal-carbon bond *trans* to a metal-amide bond were prepared as prospective new catalysts for the title reaction. Preliminary tests of catalytic activity were carried out with a palladium complex with electron withdrawing alkenyl ligand prepared by a different route. Cationic nickel(II) complexes with several diphosphinoazines which are precursors of nickel analogs to the above-mentioned pincer complexes were synthesized and factors affecting the coordination mode (square planar versus tetrahedral) were studied by the analysis of several X-ray structures determined. The X-ray structure of a palladium binuclear complex confirmed a new *(E,E)* tetracoordinated mode of diphosphinoazines. [Refs. 3, 42]

Permeable barriers with immobilized bacteria treating mixed pollutants in the environment

(G. Kuncová, joint project with ICT, supported by GA CR, grant No. 104/01/0461)

The aim of the project is to use most recent knowledge in the fields of microbiology and immobilization techniques for increasing efficiency of permeable barriers. In this project, the research will be focused on the three areas:

1) gene flow within the barriers,
2) immobilization of biomaterial by an entrapment in inorganic or organic-inorganic carriers,
3) optical sensing of polychlorinated biphenyls. [Refs. 14, 36]

International co-operations

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

Visits abroad

J. Čermák: Max-Planck-Institut für Kohlenforschung, Mülheim, Germany (2 months)

Visitors

D. Agraval, Material Research Institute, Pensylvania State University, USA

Teaching

F. Kaštánek: ICT, course "Bioengineering"

Publications

Original papers

1. Bříza T., Kvíčala J., Mysík P., Paleta O., Čermák Jan: 2-(Perfluoroalkyl)ethyl Triflates, Building Blocks for the Synthesis of Bis(polyfluoroalkylated) Cyclopentadienes. Synlett 5, 685-687 (2001).
2. Čermák Jan, Auerová K., Nguyen H.T.T., Blechta V., Vojtíšek P., Kvíčala J.: Synthesis of Rhodium Complexes with Novel Perfluoroalkyl Substituted Cyclopentadienyl Ligands. Collect. Czech. Chem.Commun. 66(2), 382-396 (2001).
3. Čermák Jan, Kvíčalová M., Šabata S., Blechta V., Vojtíšek P., Podlaha J., Shaw B.L.: Diphosphinoazines (Z,Z)-$R_2PCH_2C(But)=NN=C(But)CH_2PR_2$ with R Groups of Various Sizes and Complexes [{(Z,Z)-$R_2PCH_2C(But)=NN=C(But)CH_2PR_2$}{$\eta^3$–$CH_2C(CH_3)=CH_2$) $PdCl\}_2$]. Inorg. Chim. Acta 313, 77-86 (2001).
4. Hetflejš J., Czakóová M., Řeřicha R., Včelák J.: Catalyzed Dehalogenation of Delor 103 by Sodium Hydridoaluminate. Chemosphere 44, 1521-1529 (2001).
5. Klán P., Hájek M., Církva V.: The Electrodeless Discharge Lamp: A Prospective Tool for Photochemistry Part 3. The Microwave Photochemistry Reactor. J. Photochem. Photobiol., A 140, 185-189 (2001).
6. Zimmerman H.E., Církva V.: Excited- and Ground-State Versions of the Tri-π-methane Rearrangement: Mechanistic and Exploratory Organic Photochemistry. J. Org. Chem. 66, 1839-1851 (2001).
7. Bříza T., Kvíčala J., Paleta O., Čermák Jan: Preparation of Bis(polyfluoroalkyl)-cyclopentadienes, New Highly Fluorophilic Ligands for Fluorous Biphase Catalysis. Tetrahedron, in press.
8. Církva V., Polák R., Paleta O., Kodíček K., Forman S.: Perfluoroalkylated Derivatives of Diols and Triols. Selectivity in the Reaction of Primary and Secondary Hydroxy Groups

with Perfluoroalkylepoxides. Hemocompatibility and Effect on Perfluorocarbon Emulsion. J. Fluorine Chem., submitted.
9. Czakóová M., Hetflejš J., Včelák J.: Substituent Effects Dehalogenation of Aryl Bromides with $NaAlH_2(OCH_2OCH_3)_2$. React. Kinet. Catal. Lett. 72, 277-287 (2001).
10. Hájek M., Radoiu M.: Microwave Induced Reactions in Liquid Phase. Ceram. Trans. 111, 257-264 (2001).
11. Kaštánek F.: Zneškodňování tuhých a kapalných odpadů obsahujících PCB v synergickém systému termické, extrakční a chemické technologie. (Czech) Disposal of solid and liquid wastes containing PCBs in synergic system of thermal, extraction and chemical technology. EKO, 12, 22-25, 2001.
12. Klán P., Hájek M., Církva V.: Photochemistry in a Microwave Oven. J. Chem. Educ., submitted.
13. Kuncová G., Hetflejš J., Szilva J., Šabata S.: Immobilization of Biomaterials into Organic-Inorganic Matrices. Landbauforschung Volkenrode, submitted.
14. Kuncová G., Szilva J., Hetflejš J., Šabata S.: Catalysis in Organic Solvents with Lipase Immobilized by Sol-Gel Technique. J. Sol-Gel Sci. Technol., in press.
15. Kvíčala J., Bříza T., Paleta O., Auerová K., Čermák Jan: Synthesis, Fluorophilicities and Regioisomer Composition of Ferrocenes and Rhodium Complexes Based on Bis(polyfluoroalkylated) Cyclopentadienes. Tetrahedron, in press.
16. Marseaut S., Debourg A., Dostálek P., Votruba J., Kuncová G.: Biosorbent of Heavy Metals with Silica Matrix. Folia Microbiol., submitted.
17. Murová I., Hájek M., Lovás M.: Využitie mikrovlnnej energie pri chemickej úprave nerastných surovín. (Slov) Application of Energy in Microwave Chemical Modification of Minerals. Chem. Listy, submitted.
18. Šabata S., Hetflejš J.: Hydrogenation of Low-Molar-Mass, OH-Telechelic Polybutadienes Catalyzed by Homogeneous Ziegler Nickel Catalysts. J. Appl. Polym. Sci., in press.
19. Škvára F., Kaštánek F., Pavelková I., Šolcová O., Maléterová Y., Schneider P.: Solidification of Waste Steel Foudry Dust with Portland Cement. J. Hazard. Mater., submitted.

Chapters in books

20. Klán P., Církva V.: Microwave Photochemistry. In: Microwaves in Organic Synthesis, in press.

Patents

21. Hájek M.: Způsob a zařízení v tepelném zpracování sklářských materiálů. (Czech) Method and Equipment for Heat Treatment of glass Materials. Czech. Pat. 289 193 (2001).
22. Hájek M., Drahoš J.: Způsob a zařízení k tepelnému zpracování přírodních materiálů, zvláště vulkanického původu. (Czech) Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Vulcanic Origin. Czech. Pat. 288 978 (2001).
23. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Vulcanic Origin. PCTI/CZ00/00042/ (in press).

24. Hájek M., Volf V., Vozáb J.: Způsob a zařízení ke zpracování sklářských materiálů. (Czech) Manufacture and Equipment for Glass Material Processing. Czech. Pat. 289 191 (2001).

Conferences

25. Auerová K., Čermák Jan, Nguyen H.T.T., Blechta V.: The Synthesis of Rhodium Complexes with Cyclopentadienyl Ligands Containing Perfluoroalkyl Ponytails. 3rd International School of Organometallic Chemistry, Abstracts, pp. 39-40, Camerino, Italy, 09-13 September 2001.
26. Čermák Jan, Kvíčalová M., Auerová K., Blechta V., Vojtíšek P., Kvíčala J.: Pentamethylcyclopentadienyl Metal Complexes: From Supported Catalysts to Biphase Systems. 10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Book of Abstracts, p. 38, Lyon, France, 02-06 July 2001.
27. Chomát M., Berková D., Matějec V., Kašík I., Kuncová G., Gagnaire H., Trouillet A., Bardin F.: Optical Detection of Toluene in Water by Using IGI Fibers. Les Matériaux et leurs Applications aux Dispositifs Capteurs Physiques, Chimiques et Biologiques MADICA 2001, Recueil Des Resumes, p. A43, Hammamet, Tunisko, 29-31 October 2001.
28. Církva V., Klán P., Hájek M.: The Microwave Photochemical Reactor for Synthesis. 8th International Conference on Microwave and High Frequency Heating, Book of Abstracts, p. 97, Bayreuth, Germany, 03-07 September 2001.
29. Hájek M.: Microwave Melting Technologies. Glass Melting Technologies of the Future GMIC Workshop, Book of Abstracts, p. 2, Washington, USA, 19-22 February 2001.
30. Hájek M.: Microwave Glass Melting Technology. Conference on Application of Microwave Energy in Industry, Proceedings, p. 14, Tokyo, Japan, 30 July - 03 August 2001.
31. Hájek M.: Microwave Melting Technology. 12. Konference o elektrickém a ostatních vysoceúčinných způsobech tavení skla, Proceedings, pp. 103-106, Tábor, Czech Republic, 10-12 September 2001.
32. Kuncová G., Hetflejš J., Szilva J., Šabata S.: Immobilization of Biomaterials into Organic-Inorganic Matrices. Practical Aspects of Encapsulation Technologies, Book of Abstracts, p. 7, Braunschweig, Germany, 12-14 October 2001.
33. Kuncová G., Szilva J., Hetflejš J., Šabata S.: Catalysis in Organic Solvents with Lipase Immobilized by Sol-Gel Technique. 11th International Workshop on Glases, Ceramics, Hybrids and Nanocomposites from Gels, Abstracts, p. 225, Abano Terme, Italy, 16-21 September 2001.
34. Kuncová G., Szilva J., Hetflejš J., Šabata S.: Lipase Immobilized by Sol-Gel Technique. Bioprocess Engineering Course, Poster Abstracts, p. P-12, Supetar, Croatia, 08-14 September 2001.
35. Kuncová G., Tříska J., Vrchotová N., Podrazký O.: The Influence of Immobilization of Pseudomonas species on Optical Detection of Polychlorinated Biphenyls. Les Matériaux et leurs Applications aux Dispositifs Capteurs Physiques, Chimiques et Biologiques MADICA 2001, Book of Abstracts, p. A42, Hammamet, Tunisko, 29-31 October 2001.
36. Kuncová G., Tříska J., Vrchotová N., Podrazký O.: The Influence of Immobilization of Pseudomonas Species on the Production of Colored Metabolites. IX International BRG Workshop, Proceedings, p. P.16, Warsaw, Poland, 11-13 May 2001.
37. Kuncová G., Vaňková R., Podrazký O.: Monitoring of the Growth and Viability of Plant Cells Immobilized in Alginate Beads by Measurement of Fluorescence. IX International BRG Workshop, Proceedings, p. S.VI-1, Warsaw, Poland, 11-13 May 2001.

38. Kurfürstová J., Hájek M.: Microwave Activation of 2-tert-Butylphenol at Low Temperature. XXXIII Symposium on Catalysis, Book of Abstracts, p. 29, Praha, Czech Republic, 05-06 November 2001.
39. Kurfürstová J., Hájek M.: Microwave Activation of Catalytic Reactions at Low Temperature. 1st EFCATS School on Catalysis, Book of Abstracts, p. P26, Praha, Czech Republic, 28 March - 01 April 2001.
40. Kurfürstová J., Hájek M.: Microwave Activation of Catalytic Reactions at Low Temperature. 8th International Conference on Microwave and High Frequency Heating, Book of Abstracts, p. 269, Bayreuth, Germany, 03-07 September 2001.
41. Spirková J., Nebolová P., Mach K., Macková A., Kuncová G., Langrová A.: Copper Ion-Exchanged Optical Glass Waveguides. Les Matériaux et leurs Applications aux Dispositifs Capteurs Physiques, Chimiques et Biologiques MADICA 2001, Recueil Des Resumes, p. B36, Hammamet, Tunisko, 29-31 October 2001.
42. Storch J., Šťastná L., Galvao A.M., Čermák Jan, Carvalho M.F.N.N.: Cationic Nickel Halide Complexes with Azine Diphosphines. XIVth FECHEM Conference on Organometallic Chemistry, Book of Abstracts, p. P95, Gdansk, Poland, 02-07 September 2001.
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44. Škvára F., Kaštánek F., Pavelková I., Peřka L., Šolcová O., Schneider P.: Waste Steel Foundry Dust as Admixture in Building Materials. New Trends in Mineral technology, VŠB Ostrava, Czech Republic, 28-30 June 2001.

Department of Reaction Engineering in Gas Phase

Head: M. Punčochář
Deputy: V. Ždímal

Research groups

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

Aerosol Laboratory

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

Fields of research

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

Research projects

Composition and mode of occurrence of the mineral constituents in brown coal and thei r behaviour during fluidised bed combustion
(J. Smolík, supported by GA ASCR, grant No. A2046904)

The project is aimed at study of composition and behaviour of minerals and inorganic elements during fluidised bed combustion in connection with their distribution and mode of

occurrence. The information on modes of occurrence of elements in coal is obtained from selective leaching experiments. Special attention is also paid to the study of the effect of mineral additives on the distribution of trace elements such as As, Cd, Hg, Ni, Pb, Se, V, and Zn in emitted particles. [Refs. 31, 35]

Reduction of heavy metal emissions from fluidised bed coal combustion using sorbents
(J. Schwarz, supported by GA CR, grant No. 104/00/1297)

The project represents both experimental and theoretical effort aimed at solving important relationships in the complex processes of combustion, formation of particulate emissions, and behaviour of metal pollutants within a fluidised bed and in flue gas cleaning units. The experimental part is focused on interaction of mineral sorbets with metallic species emitted from the fluidised bed combustion of coal. Theoretical part uses thermodynamic approach to predict distribution of trace elements into different emission streams. [Refs. 31, 35]

Subgrid scale investigations of factors determining the occurrence of ozone and fine particles
(J. Smolík, supported by EC, grant No. EVK2-CT-1999-00052 SUB-AERO)

Objective of the project is the understanding of the formation, accumulation, fate, and effects of ozone, other photochemical oxidants and fine particulate matter in subgrid ("local") scale in the Mediterranean area. This is accomplished by incorporating state-of-the-art field measurements combined with the state-of-the-art analysis/mesoscale-subgrid modelling tools, which improve quantification of the relationships between emission source activity and ambient air quality for photochemical pollutants and fine particles. [Refs. 16, 17, 20, 23]

Characterization of urban air quality – indoor/outdoor particulate matter chemical characteristics and source-to-inhaled dose relationships
(J. Smolík, supported by EC, grant No. EVK4-CT-00018 URBAN-AEROSOL)

The project aims: i) to characterize chemically the particulate matter associated with actual human exposure in selected residential European areas, ii) to provide an integrated European exposure assessment database for urban PM characterization through indoor/outdoor monitoring and modelling, iii) to study and evaluate the mechanisms controlling the indoor/outdoor relationships of PM by taking into account infiltration, meteorological conditions, indoor sources of PM, physical and chemical processes indoors, and the composition/size distribution of indoor generated particulate matter, by using mechanistically based models, and iv) to link human exposure to particulate matter indoor with physiologically based mechanistic dosimetry models. [Ref. 19]

Physicochemical properties of urban atmospheric aerosol. Source apportionment and impact on air quality
(J. Smolík, supported by AIE CR, grant No. KONTAKT 25)

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

International co-operations

Philipps-University of Marburg, Marburg, Germany: Experimental study of homogeneous nucleation in supersaturated vapours
University of Helsinki, Helsinki, Finland: Condensation processes as a part of gas-to-particle conversion
Finnish Meteorological Institute, Helsinki, Finland: Application of cascade impactors for aerosol studies
Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece: Urban aerosols
Norwegian Institute for Air Research, Kjeller, Norway: Formation of ozone and fine particles in the Mediterranean area
University of Essex, Colchester, U.K.: Sampling of fine atmospheric particles
Institute for Systems, Informatics and Safety, JRC-Ispra, Italy: Modelling of fine particle formation
Technical University of Crete, Greece: Aerosols in the environment
Fraunhofer Institute ITA, Germany: Indoor/outdoor aerosols

Visitors

P. E. Wagner, University of Vienna, Vienna, Austria
G. Kiss, Air chemistry group of the Hungarian Acad. Sci., Veszprém, Hungary

Publications

Original papers

1. Bakanov S.P., Smolík J., Zaripov Sh.Kh., Ždímal V.: Continuum Regime Motion of a Growing Droplet in Opposing Thermo-Diffusiophoretic and Gravitational Fields of a Thermal Diffusion Cloud Chamber. J. Aerosol. Sci. 32, 341-350 (2001).
2. Levdansky V.V., Kim H.Y., Kim H.C., Smolík J., Moravec P.: Effect of Electromagnetic Fields on Transfer Processes in Heterogeneous Systems. Int. J. Heat Mass Transfer 44(5), 1065-1071 (2001).
3. Levdansky V.V., Smolík J.: Kinetika fizicheskogo i khimicheskogo osazhdeniay vestestva iz gazovoi fazy v kanalakh. (Russ) Kinetics of Physical and Chemical Deposition of Substance from Gas Phase in Channels. Inzh.-Fiz. Zh. 74(5), 142-145 (2001).
4. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Vliyanie poverkhnostnykh yavlenii na rost aerozolnykh chastits v bufernom (primesnom) gaze. (Russ) Influence of Surface Phenomena on the Growth of Aerosol Particles in Buffer (Admixture) Gas. Inzh.-Fiz. Zh. 74(4), 138-140 (2001).
5. Moravec P., Smolík J., Levdansky V.: Preparation of TiO_2 Fine Particles by Thermal Decomposition of Titanium Tetraisopropoxide Vapor. J. Mater. Sci. Lett. 20(22), 2033-2037 (2001).
6. Moravec P., Smolík J., Levdansky V.V.: Preparation of Fine Particles by Decomposition of Aluminum Tri-Sec-Butoxide Vapor. J. Mater. Sci. Lett. 20, 311-313 (2001).

7. Smolík J., Džumbová L., Schwarz J., Kulmala M.: Evaporation of Ventilated Water Droplet: Connection Between Heat and Mass Transfer. J. Aerosol. Sci. 32(6), 739-748 (2001).
8. Stratmann F., Wilck M., Ždímal V., Smolík J.: 2-D Model for the Description of Thermal Diffusion Cloud Chambers: Description and First Results. J. Phys. Chem. B 105(47), 11641-11648 (2001).
9. Uchtmann H., Kazitsyna S.Yu., Hensel F., Ždímal V., Tříska B., Smolík J.: Homogeneous and Light-Induced Nucleation of Sulfur Vapor-Diffusion Cloud Chamber Investigation of Constant Rate Supersaturation. J. Phys. Chem. B 105(47), 11754-11762 (2001).
10. Bakanov S.P., Ždímal V., Zaripov Sh.Kh., Smolík J.: Matematicheskaya modeľ dvizheniya aerozoľnykh chastits v termodifuzionnoi kamere. (Russ) Mathematical Model of Motion of Aerosol Particles in a Thermal Diffusion Cloud Chamber. Colloidn. Zh., submitted.
11. Levdansky V.V., Smolík J., Moravec P., Ždímal V.: Khimicheskoe osazhdenie na aerozol'nykh chastitsakh. (Russ) Chemical Deposition on Aerosol Particles. Inzh.-Fiz. Zh., submitted.
12. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Growth and Evaporation of Aerosol Particles in the Presence of Adsorbing Gases. Int. J. Heat Mass Transfer, submitted.
13. Maenhaut W., Schwarz J., Cafmeyer J., Annegarn H.J.: Study of Elemental Mass Distributions at Skukuza, South Afrika, during the SAFARI 2000 Dry Season Campaign. Nucl. Instrum. Methods Phys. Res., Sect B, submitted.
14. Maenhaut W., Schwarz J., Cafmeyer J., Chi X.: Aerosol Chemical Mass Closure during the EUROTRAC-2 AEROSOL Intercomparison 2000. Nucl. Instrum. Methods Phys. Res., Sect B, in press.

Conferences

15. Bakanov S.P., Ždímal V., Zaripov Sh.Kh., Smolík J.: Dvizhenie aerozol'nykh chastits v termodiffuzionnoi kamere. (Russ) Motion of Aerosol Particles in a Thermal Diffusion Cloud Chamber. 8th All-Russian Meeting on Theoretical and Applied Mechanics, Proceedings, p. 67, Perm, Russia, 23-29 August 2001.
16. Colbeck I., Bryant C., Drossinos I., Havránek V., Mikuška P., Smolík J., Večeřa Z., Ždímal V., Eleftheriadis K., Housiadas C., Lazaridis M., et al.: Preliminary Results from Subgrid Scale Investigations of Factors Determining the Occurrence of Ozone and Fine Particles (SUB-AERO). Aerosol Society Annual Meeting, Book of Abstracts, pp. 12-15, University of Bath, Great Britain, 18-19 June 2001.
17. Colbeck I., Bryant C., Nyeki S., Eleftheriadis K., Smolík J., Ždímal V., Lazaridis M., Mihalopoulos N.: Optical Properties of Atmospheric Aerosol at Finokalia (Greece). European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S445 (2001)], Leipzig, Germany, 03-07 September 2001.
18. Havránek V., Voseček V., Kučera J., Smolík J., Schwarz J.: Analysis of Different Aerosol Samples from Cascade Impactors by Pixe – Efficiency Calibration and Matrix Effects. 12th International Symposium Spectroscopy in Theory and Practice, Book of Abstracts, p. 31, Bled, Slovenia, 09-12 April 2001.
19. Lazaridis M., Asimakopoulos D.N., Braniš M., Colbeck I., Drossinos I., Dye C., Eleftheriadis K., Flocas H., Helmis C., Hollander W., Smolík J., Ždímal V.: Characterisation of Urban Air Quality Indoor/Outdoor Particulate Matter Chemical Characteristics and Source-to-Inhaled Dose Relatioships (Urban-Aerosol). European

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20. Lazaridis M., Colbeck I., Drossinos I., Eleftheriadis K., Havránek V., Kallos G., Smolík J., Solberg S., Spiridaki A., Stefanou E., Večeřa Z., Ždímal V.: Subgrid Scale Investigations of Factors Determinating the Occurrence of Ozone and Fine Particles (SUB-AERO). European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S119-S120 (2001)], Leipzig, Germany, 03-07 September 2001.
21. Lazaridis M., Colbeck I., Drossinos I., Eleftheriadis K., Havránek V., Housiadas C., Kallos G., Mikuška P., Smolík J., Večeřa Z., Ždímal V., et al.: Subgrid Scale Investigations of Factors Determining the Occurrence of Ozone and Fine Particles (SUB-AERO). 8th European Symposium on the Physico-Chemical Behaviour of Atmospheric Pollutants, Abstracts, p. AP86, Torino, Italy, 17-20 September 2001.
22. Levdansky V.V., Smolík J., Moravec P.: Coating of Small Particles by Films. The European Material Conference E-MRS 2001 Spring Meeting, Book of Abstracts/ Resumes, p. C-25, Strasbourg, France, 05-08 June 2001.
23. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Effect of Foreign (Buffer) Gases on Deposition Processes in Aerosol Systems. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S575-S576 (2001)], Leipzig, Germany, 03-07 September 2001.
24. Maenhaut W., Cafmeyer J., Chi X., Schwarz J.: Assessment of Artifacts in Filter Collections for Carbonaceous Aerosol and the Particulate Mass. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S673-S674 (2001)], Leipzig, Germany, 03-07 September 2001.
25. Maenhaut W., Schwarz J., Cafmeyer J., Annegarn H.J.: Study of Elemental Mass Size Distribution at Skukuza, South Afrika, during the SAFARI 2000 Dry Season Campaign. IX International Conference on Particle-Induced X-Ray Emission and its Analytical Applications PIXE 2001, Appendix, p. 96, Guelph, Canada, 08-12 June 2001.
26. Maenhaut W., Schwarz J., Cafmeyer J., Chi X.: Aerosol Chemical Mass Closure during the EUROTRAC-2 AEROSOL Intercomparison 2000. IX International Conference on Particle-Induced X-ray Emission and its Analytical Applications PIXE 2001, Appendix, p. 34, Guelph, Canada, 08-12 June 2001.
27. Maenhaut W., Schwarz J., Cafmeyer J., Chi X.: Chemical Mass Closure during the EUROTRAC-2 AEROSOL Intercomp 2000. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S1017-S1018 (2001)], Leipzig, Germany, 03-07 September 2001.
28. Maenhaut W., Schwarz J., Cafmeyer J., Chi X.: Particulate Mass and Organic and Elemental/Black Carbon during the EUROTRAC-2 AEROSOL Intercomp 2000. Eurotrac-Aerosol-Workshop, Abstracts, Cologne, Italy, 21-22 March 2001.
29. Müller K., Spindler G., Brüggeman E., Gnauk T., Koziar Ch., Schwarz J., Cafmeyer J., Maenhaut W., Even A., Kok J., Berner A., Ctyroky P.: The Experiment "Intercomp 2000" in Melpitz - an EUROTRAC-2 Activity. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S1021-S1022 (2001)], Leipzig, Germany, 03-07 September 2001.
30. Petrova T., Semkov K., Moravec P.: Determining the Characteristic Size of the Packing in the Mathematical Model Describing Spreading of the Liquid in Packed Bed Columns with Wall Flow Deflecting Rings. 9th International Summer School of Chemical Engineering, Proceedings, p. 63, Sozopol, Bulgaria, 18-24 September 2001.
31. Schwarz J., Smolík J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate Emissions from Fluidized Bed Combustion of Lignite with and without

Recirculation. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S27-S28 (2001)], Leipzig, Germany, 03-07 September 2001.
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34. Smolík J., Ždímal V., Wagner Z., Eleftheriadis K., Lazaridis M., Colbeck I.: Submicrometer Particle Number Size Distributions of Atmospheric Aerosol in the Mediterranean Area. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S145-S146 (2001)], Leipzig, Germany, 03-07 September 2001.
35. Sýkorová I., Vašíček, M., Smolík J., Schwarz J., Džumbová L., Machovič V., Kučera J., Havránek V.: Solid Emissions from the Atmospheric Fluidized Bed Combustion of Lignite. 11th International Conference on Coal Science, San Francisko, USA, 30 September - 05 October 2001.
36. Uchtmann H., Kazitsyna S.Yu., Hensel F., Ždímal V., Tříska B., Smolík J.: Homogeneous and Light-Induced Nucleation of Sulfur Vapor. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S11-S12 (2001)], Leipzig, Germany, 03-07 September 2001.

Group of Hydrodynamics and Chemistry of Incineration

Research staff: M. Punčochář, E. Fišerová, J. Nesvadbová, V. Pekárek, V. Tydlitát
Technical staff: P. Hájek, J. Ullrich
PhD student: M. Jochová, S. Chytil

Fields of research

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

Applied research

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

Research projects

Power combustion of wastes and biomass
(M. Punčochář, supported by GA CR, grant No. 104/97/S002)

Experiments were done on the 100 kW CFB reactor with combustion of lignite, charcoal, and, as a source of chlorine, PVC powder was added in some experiments. The effect of sulfur compounds (diluted and concentrated sulfuric acid, sulfur dioxide with hydrogen peroxide) was explored for the reduction of polyhalogenated dibenzo-p-dioxins and benzofuran emissions. The most efficient additives for PCDD/F dropping, that we found, were the concentrated H_2SO_4 and the combination SO_2+H_2O_2. The application of concentrated sulfuric acid depended strongly on the temperature in the place where the acid was applied. Big difference between application of diluted and concentrated acid were found in concentrations of PCDD on fly ash. The concentrated acid is much more efficient for removing of PCDD/F. We found that the different experience with influence of SO_2 in flue gas on PCDD/F formation is probably due to the equilibrium $SO_3 \leftrightarrow SO_2$. The strong correlation between concentration of dioxins and level of O_2 in flue gas was also experimentally proved. [Refs. 3, 4, 11, 13]

Detoxification of polyhalogenated dibenzo-p-dioxins and benzofurans on catalytically active surfaces of inorganic sorbents
(V. Pekárek, supported by GA ASCR, grant No. A4072901)

The fly ashes from municipal waste incinerators contain significant amounts of persistent organic pollutants from which the dioxins and benzofurans are of the highest chemical stability and toxicity. Their detoxification by means of dehalogenation on catalytically active surfaces was therefore studied. It was found that the dehalogenation efficiency of ash depends on the quality of skeleton, presence of metals, amount and chemical form of carbon and on the reaction conditions. A synthetic analogue of ash was created for optimal dehalogenation. Using this synthetic ash, HCB was totally converted to benzene and Delor 103 to biphenyl. A mixed batch reactor was built for dehalogenation of PCB in waste oil. Further, experiments were done for explanation of SO_2, H_2O_2 and H_2SO_4 influence on the course of novosynthetic reactions in the system extracted ash, $CuCl_2.2H_2O$, and NaCl at 340 ^oC. [Ref. 1, 5, 8, 9, 12]

Cleaning of underground water by coal based sorbents
(M. Punčochář, supported by Grant Agency of Ministry of Environment, grant No. VaV 550/1/99)

Calcium loaded coal is used for removing heavy metals and organic pollutants from underground water. Lignite loaded by calcium is an effective ion-exchanger. Coal with metal and organic pollutants is combusted in a fluidized bed with simultaneous capture of fly ash and flue gas pollutants. A model was developed for prediction of ion exchange in coal. The technology was verified in the long-term pilot plant experiment [Ref. 10]

International co-operations

NIRE, Tsukuba, Japan: Metals recycling
Vrije Universiteit Brussels, Belgium: Formation of POPs
Forschungzentrum Karlsruhe, Institut fűr Technische Chemie, Karlsruhe, Germany: Dioxin chemistry

Visitors

L. Stieglitz, Forschungzentrum Karlsruhe, Institut fűr Technische Chemie, Karlsruhe, Germany

Publications

Original papers

1. Pekárek V., Grabic R., Marklund S., Punčochář M., Ullrich J.: Effects of Oxygen on Formation of PCB and PCDD/F on Extracted Fly Ash in the Presence of Carbon and Cupric Salt. Chemosphere 43, 777-782 (2001).
2. Drahoš J., Punčochář M.: Comments on Application of the Fractional Brownian Motion in an Airlift Reactor. Chem. Eng. Sci., in press.
3. Grabic R., Pekárek V., Ullrich J., Punčochář M., Fišerová E., Šebestová M.: Effect of Reaction Time on PCDD and PCDF Formation by De-novo Synthetic Reactions under Oxygen Defficient and Rich Atmosphere. Chemosphere, submitted.
4. Pekárek V., Grabic R., Punčochář M., Ullrich J., Fišerová E., Bureš M.: Effect of Sulphur Dioxide, Hydrogen Peroxide, Sulphuric Acid and Their Mictures on the De-novo Synthesis of PCDD and PCDF in the N_2 + 10% O_2 Atmosphere Under Model Laboratory Conditions. Chemosphere, submitted.
5. Pekárek V., Karban J., Fišerová E., Bureš M., Pacáková V., Večerníková E.: Why the Fly Ash Acts as the Dehalogenating Agent? Environ. Sci. Technol., submitted.
6. Tydlitát V., Pekárek V., Janota J.: Emise toxických složek při spalování použitých motorových olejů v hořákovém kotli 102 kW. (Czech) Emissions of Toxic Components from Waste Engine Oils Combustion in the 102 kW Boiler with the Atomizing Burner. Ochrana Ovzduší, in press.

Chapters in books

7. Drahoš J., Punčochář M.: Fraktály a chaos: Věda o běžných věcech. (Czech) Fractals and Chaos: Science about Common Matters. In: Vybraná témata na přelomu tisíciletí. (Czech). (Mareš, M, Nekola, J., Řeřicha, R., Eds.), pp. 33-45, Česká asociace Římského klubu, Praha 2001.

Patents

8. Pekárek V., Hapala P., Fišerová E.: Způsob dehalogenace halogenovaných aromatických sloučenin. (Czech) Method of Aromatic Halogenated Compounds Dehalogenation. Pat. No. PV 2001-4370. Applied: 01.12.05.

Conferences

9. Bureš M., Pekárek V., Fišerová E.: Katalytická dehalogenace hexachlorobenzenu na modelovém a extrahovaném popílku v porovnání s termodynamickou interpretací dechloračního procesu. (Czech) Catalytic Dehalogenation of Hexachlorobenzene by Model and Extracted MSWI Fly Ash in Comparison with Thermodynamical Interpretation of the Dechlorination Process. Mezinárodní slovenský a český kalorimetrický seminář 2001, Sborník příspěvků, pp. 35-37, Račkova Dolina - Pribylina, Slovakia, 28 May - 01 June 2001.
10. Jochová M., Horáček J., Punčochář M.: Cleaning of Underground Water by Coal Based Sorbents. 28th International Conference of Slovak Society of Chemical Engineering, Book of Abstracts, p. 89, Tatranské Matliare, Slovakia, 21-25 May 2001.
11. Pekárek V., Grabic R.: The Effect of Time on PCDD/F, PCBs Formation under Oxygen Deficient and Rich Atmosphere. Karasek Meeting, Durbuy/Brussels, Belgium, 29 April - 03 May 2001.
12. Pekárek V., Grabic R.: The Effect of the Matrix and Oxygen on PCDD/F, PCBs Formation. Karasek Meeting, Durbuy/Brussels, Belgium, 29 April - 03 May 2001.
13. Punčochář M., Veselý V., Grabic R., Tydlitát V., Pekárek V.: The Combustion Conditions and PCDD/F Emissions. 6th International Conference on Technologies and Combustion for a Clean Environment, Volume 2, pp. 757-761, Oporto (Porto), Portugal, 09-12 July 2001.

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

Research staff: M. Hartman, Ji. Čermák, K. Svoboda, O. Trnka, V. Veselý
Technical staff: J. Chour, M. Pohořelý

Fields of research

- Gas-solid reactions
- Gas-solid reactors and operations
- Fluidized bed combustion
- Gaseous and particulate emissions from combustion and industrial processes
- Solid waste treatment and co-combustion

Research projects

Reaction and reactors for hot coal-gas desulphurization with calcareous materials
(M. Hartman, supported by GA ASCR, grant No. A4072711)

Possibilities of using various calcareous materials are explored for hot coal-gas desulphurization. Practical reaction rate equations are developed and incorporated into tractable models of the reactors for contacting coal-gas with solid sorbents. [Refs. 5, 6, 9, 10]

Pressurized fluidized bed combustion of coal, emissions of nitrogen oxides and effect of biomass addition to the fuel on emissions and behaviour of the pressurized fluidized bed under combustion conditions
(K. Svoboda, supported by GA ASCR, grant No. A4072801)

The project in the field of Clean Coal Technology and biomass-co-combustion is concentrated on experimental investigation and modelling of pressurized bed combustion of coal and biomass-coal blends. Target of the research work: emissions (NO_x, N_2O, CO, SO_2), maximum particle temperature and agglomeration of coal/biomass-ash particles. [Refs. 1, 6, 8, 9, 13]

Low emissions with extremely staged (pressurized) coal combustion - A novel concept
(K. Svoboda, supported by the EC in the program INCO-Copernicus, Contract No. ERBIC15-CT98-0513)

The project, with its experimental and theoretical part, is focused on differences between oxidizing, slightly reducing and air stagging conditions in the pressurized fluidized bed combustion of selected coals on overall emissions, (esp. NO, N_2O, SO_x) in modern coal combined cycle power generation. [Refs. 1, 7, 11, 16]

Evaluation of dynamic states of gas fluidized suspensions via pressure fluctuations
(O. Trnka, supported by GA ASCR, grant No. A4072001)

Research is oriented on developing new tools for the on-line diagnostics of flow regimes in fluidized beds. Pressure fluctuations within the beds are measured and subjected to detailed analysis. Novel and rigorous computational procedures are developed for the evaluation of pressure fluctuation time series. [Refs. 9, 12]

International co-operations

University College London, London, UK: High temperature fluidization
University of Connecticut, Storrs, USA: Desulfurization of Gases
Delft University of Technology, Delft, The Netherlands: Circulating fluidized beds
Technical University Cottbus, Germany: Pressurized fluidized bed combustion
Institute of Physical Chemistry, PAS, Warsaw, Poland: Fluidized bed operations
ECN Petten, The Netherlands: Pressurized fluidized bed combustion/gasification technologies

Visitors

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

Teaching

M. Hartman: ICT, postgraduate course "Multiphase reactors"
K. Svoboda: ICT, course "Environmental engineering"

Publications

Original papers

1. Čermák Ji., Svoboda K., Pohořelý M.: Zkušenosti s použitím analyzátoru FTIR k analýze spalin. (Czech) Application of FTIR Analyser to Analyse Waste Gases. AUTOMA 7(10), 12-15 (2001).
2. Hartman M., Trnka O., Veselý V., Svoboda K.: Thermal Dehydration of the Sodium Carbonate Hydrates. Chem. Eng. Commun. 185, 1-16 (2001).
3. Hartman M., Veselý V., Svoboda K., Trnka O., Beran Z.: Dehydration of Sodium Carbonate Decahydrate to Monohydrate in a Fluidized Bed. AIChE J. 47(10), 2333-2340 (2001).
4. Hartman M., Trnka O., Veselý V., Svoboda K.: Properties of Sodium Carbonates Beds at Incipient Fluidization and Terminal Velocities of Solids. Chem. Pap. 55(3), 149-153 (2001).
5. Hartman M., Svoboda K., Trnka O.: Comments on "Design of Entrained-Flow and Moving-, Packed-, and Fluidized-Bed Sorption Systems: Grain-Model Kinetics for Hot Coal-Gas Desulfurization with Limestone". Ind. Eng. Chem. Res., submitted.
6. Hartman M., Svoboda K., Trnka O., Čermák Ji.: Reaction between Hydrogen Sulfide and Limestone Calcines. Ind. Eng. Chem. Res., submitted.
7. Svoboda K., Hartman M., Čermák Ji., Pohořelý M.: Desulfurization under Conditions of Substoichiometric Pressurized Fluidized Bed Combustion of Coal – Comparison with TG-Tests and Equilibrium Limits. Acta Montana, Ser. B, 120(11), 39-53 (2001).
8. Svoboda K., Hartman M., Čermák Ji.: Effect of Pressure and Temperature on Coal Behaviour in PFBC/G. Acta Montana, Ser. B, submitted.

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9. Hartman M., Trnka O., Svoboda K., Veselý V.: Turbulentní fluidace. (Czech) Turbulent Fluidization. Chem. Listy 95, 556-562 (2001).
10. Hartman M., Svoboda K., Trnka O., Veselý V.: Reakce vápenatých a hořečnatých materiálů při vysokoteplotním odsiřování spalin a energetického plynu. (Czech) Reactions of Calcareous and Magnesian Compounds in the Desulfurization of Flue and Coal Gas at High Temperature. Chem. Listy, submitted.

Patents

11. Svoboda K., Čermák Ji., Hartman M., Baťalík J., Gubčo V.: Způsob energetického využití tuhých paliv s tlakovým zplyňováním a paro-plynovým cyklem a zařízení k jeho provádění. (Czech) Method and Apparatus for Solid Fuel Pressurized Gasification with Combined Cycle Power Generation. Czech. Pat. Appl. PV 2001 - 1039.
12. Veselý V., Trnka O., Hartman M.: Způsob řízení a identifikace režimů fluidní vrtstvy zrnitého materiálu. (Czech) Control and Identification of a Regime of the Fluidized Bed. Pat. No. PV 314-99. Applied: 01.04.01.

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13. Čermák Ji., Svoboda K., Pohořelý M.: Pressurized Substoichiometric Combustion of Coal. 28th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 112, Tatranské Matliare, Slovakia, 21-25 May 2001.
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15. Schwarz J., Smolík J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate Emissions from Fluidized Bed Combustion of Lignite with and without Recirculation. European Aerosol Conference EAC 2001, Book of Abstracts [in J. Aerosol. Sci., 32 (Suppl. 1), S27-S28 (2001)], Leipzig, Germany, 03-07 September 2001.
16. Svoboda K., Čermák Ji., Hartman M., Pohořelý M.: Low Emissions with Extremly Staged Coal Combustion – Substoichiometric Combustion and Desulfurization at 800 °C. INCO-Copernicus Final Meeting, Book of Abstracts, Brussels, Belgium, 15 January 2001.

Laser Chemistry Group

Research staff: J. Pola, V. Dřínek, R. Fajgar, A. Galík, A.Galíková, J. Kupčík, D. Pokorná, M. Urbanová, K. Vacek
NATO fellow: R. Tomovska
PhD student: K. Jursíková

Fields of research

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

Research projects

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

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

IR laser photolysis of 1,1,1,3,3,3-hexamethyl-2,2-divinyl-trisilane and IR laser ablation of dodecamethylcyclohexasilane has been examined to show behaviour of these polysilanes under intense laser light. Both reactions result in the deposition of organosilicon films.

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

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

IR laser thermolysis of silacyclopent-3-ene results in extrusion of silylene and can serve as efficient method for chemical vapour deposition of polycarbosilane films produced via reactions of silylene, butadiene and methylene. ArF laser photolysis of silacyclopent-3-ene is interfered in the presence of alcohols, carboxylic acid and oxygen but not in the presence of carbon oxides, the interference being interpreted in terms of reactions of silylene with the admixtures. IR laser thermolysis of (chloromethyl)silane takes place as 1,1- HCl elimination and dehydrogenation and results in chemical vapour deposition of nanostructured Si/C/H phases. [Ref. 17]

Laser ablation and chemistry of silicon monoxide

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

IR laser ablation of silicon monoxide [Ref. 2] in the absence and presence of gaseous water, hydrogen, carbon monoxide and methanol [Ref. 18] has been studied to explore reactivity of ablated particles towards these compounds. The films obtained via reactions of silicon monoxide with the above molecules were characterized by FTIR and XP spectroscopy and electron microscopy. They are composed of different $Si_xO_yH_z$ configurations, contain both Si-H and Si-OH bonds and can be suitable precursors for fabrication of organically-modified SiO_x materials. Pulsed laser ablation of bulk poly[oxy(tetramethyldisilane-1,2-diyl)] affords [Ref. 21] thin films of intractable hybrids of siloxanes and polysilylenes which are thermally superior to siloxanes and polysilylenes. They are promising for applications in thermally exposed devices. [Ref. 6]

Laser induced decomposition of hydridosiloxanes

(J. Pola, supported by Ministry of Education, Program KONTAKT)

IR laser decomposition of hydridosiloxanes and reactions of hydridosiloxanes with Cl atoms has been studied [Refs. 5, 12, 15, 16, 19, 20]. The results show that the reactivity of the Si-H bond in disiloxanes towards Cl is higher than that of the C-H bond. Both systems afford polymeric deposits, which were characterized by spectral methods and electron microscopy.

Laser photolysis and thermolysis of organic and organometallic compounds for fabrication of nano-structures of metals in polymer matrices

(J. Pola, supported by GAAV CR, grant No. A 4072107)

IR laser gas-phase co-pyrolysis of iron pentacarbonyl and silacyclic compounds results in unusual polymerisation of the silacycles affording Fe clusters enveloped by organosilicon polymer. UV laser photolysis of diethyl selenium and tellurium occurs via molecular elimination of ethane and yields thin films of elemental selenium and tellurium [Refs. 8-11]. UV laser photolysis of acetylene can be used for chemical vapour deposition of saturated polyalkane polymer films.

Laser induced deposition of naked and polymer-embedded metal clusters

(J. Pola, supported by Ministry of Youth and Sports, Program COST, grant No. OC 523.60)

UV laser photolysis of 1,3-disilacyclobutane in molecular oxygen occurs via oxidation of transient silene and affords nanostructured polyoxocarbosilane films poor in hydrogen [Ref. 14]. Laser-induced gas-phase photolysis of unsaturated organylsilanes is a feasible method of polymerisation of these compounds and affords thin films of organosilicon polymers [Refs. 7, 13]. UV laser gas-phase co-photolysis of tetravinylgermane and carbon disulfide affords chemical vapour deposition of organogermanium films that are produced by co-polymerization of both reactants. UV laser photolysis of gaseous trimethoxysilane yields ultrafine powders of SiO_x materials with low content of carbon and shows an effective removal of carbon moieties from the reactant.

International co-operations

CEA-DSM-DRECAM, Service des Photons, Atomes et Molecules, Saclay, France
Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lódź, Poland
Chiba University, Japan: Laser-induced production of novel organosilicon polymers
Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of polycarbosilanes and silicon carbide
Institute of Spectroscopy, RAS, Troitsk, Russia: IR photolysis of silacycles in the condensed state
National Institute of Materials and Chemical Research, Tsukuba, Japan: Laser control of organic reactions
Technical University, Graz, Austria: Laser chemistry of polysilanes
University of Crete, Heraklion, Greece: Infrared multiphoton photolysis of disiloxanes

Visits abroad

V. Dřínek: Institute of Materials and Chemical Research, Tsukuba, Japan (3 months)
J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (2 months)
J. Pola: Chiba University, Japan (1 month)

Visitors

H. Morita, Chiba University, Japan
L. Tumanova, Institute of Spectroscopy, Troitsk, Russia
E. A. Volnina, Institute of Petrochemical Research, Moscow, Russia
N. Herlin, CEA-DSM-DRECAM, Service des Photons, Atomes et Molecules, Saclay, France
F. Tenegal, CEA-DSM-DRECAM, Service des Photons, Atomes et Molecules, Saclay, France
P. Papagiannakopoulos, University of Crete, Heraklion, Greece

Publications

Original papers

1. Dřínek V., Niino H., Pola J., Yabe A.: Surface Modification of a Polymer Film by Cryogenic Laser Ablation of Organosilicon Compounds. Appl. Phys. A 73, 527-530 (2001).
2. Dřínek V., Pola J., Bastl Z., Šubrt J.: TEA CO_2 Pulsed Laser Deposition of Silicon Suboxide Films. J. Non-Cryst. Solids 288, 30-36 (2001).
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4. Galíková A., Galík A.: Gravimetric Study of the Dynamics of Adsorption, Desorption and of Polymerization of Propene on γ- Alumina. Chem. Pap. 55(6), 397-400 (2001).
5. Kupčík J., Bastl Z., Šubrt J., Pola J., Papadimitrou V.C., Prosmitis A.V., Papagiannakopoulos P.: IR Laser-Induced Decomposition of Hexamethyldisiloxane for Chemical Vapour Deposition of Nano-Structured Hydrido(Methyl)Silicone Powders. J. Anal. Appl. Pyrolysis 57, 109-118 (2001).
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9. Pola J., Bastl Z., Šubrt J., Ouchi A.: Atmospheric Pressure Chemical Vapour Deposition of Selenium and Tellurium Films by UV Laser Photolysis of Diethyl Selenium and Diethyl Tellurium. Appl. Organometal. Chem 15, 924-930 (2001).
10. Pola J., Bastl Z., Šubrt J., Ouchi A.: Atmospheric Pressure Chemical Vapour Deposition of Selenium Films by KrF Laser Photolysis of Dimethyl Selenium. Appl. Surf. Sci. 172, 220-224 (2001).
11. Pola J., Ouchi A.: UV Laser-Induced Photolysis of Diethyl Selenium and Diethyl Tellurium: Extrussion of Selenium and Tellurium via Molecular Elimination of Ethene. J. Organomet. Chem. 629, 93-96 (2001).
12. Pola J., Ouchi A., Bastl Z., Šubrt J., Sakuragi M., Galíková A., Galík A.: UV Laser Photodeposition of Nanotextured Poly(hydridomethylsiloxane) Powder from Gaseous 1,3-Dimethyldisiloxane. Chem. Vap. Deposition 7(1), 19-22 (2001).
13. Pola J., Urbanová M., Bastl Z., Šubrt J., Sakuragi M., Ouchi A., Morita H.: Laser-Induced Formation of Polymers from Unsaturated (Organyl)Trimethylsilanes in the Gas Phase. Polymer 42, 1311-1318 (2001).
14. Pola J., Vítek J., Bastl Z., Šubrt J.: UV Laser-Induced Photolysis of 1,3-Disilacyclobutane in Oxygen for Chemical Vapour Deposition of Nano-Sized Polyoxocarbosilane Films. J. Organomet. Chem. 640, 170-176 (2001).
15. Prosmitis A.V., Papadimitriou V.C., Pola J., Papagiannakopoulos P.: Kinetic Study for the Reactions of Chlorine Atoms with Hexamethyldisiloxane, 1,1,3,3-Tetramethyldisiloxane, and 1,3-Dimethyldisiloxane. Chem. Phys. Lett. 344, 241-248 (2001).
16. Urbanová M., Bastl Z., Šubrt J., Pola J.: IR Laser-Induced Thermolysis and UV Laser-Induced Photolysis of 1,3-Diethyldisiloxane: Chemical Vapour Deposition of Nanotextured Hydridoalkylsilicones. J. Mater. Chem. 11, 1557-1562 (2001).
17. Urbanová M., Pola J.: Infrared Laser-Powered Homogeneous Decomposition of (Chloromethyl)trimethylsilane: 1,2-Cl Shift and Methene Expulsion Yielding Chlorotrimethylsilane. J. Anal. Appl. Pyrolysis 62(2), 197-203 (2001).

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19. Herlin-Boime N., Ténégal F., Bastl Z., Šubrt J., Jursíková K., Blechta V., Pola J.: IR Laser Thermolytic Conversion of Disiloxanes to Polyoxocarbosilane Phase and Silicon Carbide. J. Mater. Chem., submitted.
20. Pola J., Galíková A., Galík A., Bastl Z., Šubrt J., Ouchi A., Sakuragi M.: UV Laser Photolysis of Disiloxanes for Chemical Vapour Deposition of Nano-Textured Silicones. Chem. Mater., in press.
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Department of Analytical Chemistry

Head: J. Schraml
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Technical staff: J. Lněničková

Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

Applied research

- Analytical services to the research departments of ICPF

Research projects

^{29}Si NMR chemical shifts
(J. Schraml, supported by GA CR, grant No. 203/99/0132)

A continued study of electronic and steric effects on the NMR chemical shifts of ^{29}Si and their utilization in the analysis of complex systems. [Refs. 5, 14]

Structure and spectra of hydroxamic acids and their derivatives under various conditions
(J. Schraml, supported by GA AS CR, grant No. A4072005)

Spectral studies of derivatives of hydroxamic acids under different experimental conditions and states of matter with the aim of determining the dependence of their structure on the environmental conditions. [Refs. 10, 12]

International co-operations

University of Ghent, Ghent, Belgium: Study of Neurotoxins as Food Contaminants
Catholic University of Leuven, Leuven, Belgium: NMR in medicinal chemistry
Institute of Organic Chemistry, BAS, Sofia, Bulgaria: Dynamic NMR

Teaching

J. Schraml: CU and ICT, course "NMR Spectroscopy"

Publications

Original papers

1. Čermák Jan, Auerová K., Nguyen H.T.T., Blechta V., Vojtíšek P., Kvíčala J.: Synthesis of Rhodium Complexes with Novel Perfluoroalkyl Substituted Cyclopentadienyl Ligands. Collect. Czech. Chem. Commun. 66(2), 382-396 (2001).
2. Čermák Jan, Kvíčalová M., Šabata S., Blechta V., Vojtíšek P., Podlaha J., Shaw B.L.: Diphosphinoazines (Z,Z)-$R_2PCH_2C(But)=NN=C(But)CH_2PR_2$ with R Groups of Various Sizes and Complexes [{(Z,Z)-$R_2PCH_2C(But)=NN=C(But)CH_2PR_2$}{$\eta^3$–$CH_2C(CH_3)=CH_2$) $PdCl\}_2$]. Inorg. Chim. Acta 313, 77-86 (2001).
3. Karban J., Buděšínský M., Černý M., Trnka T.: Synthesis and NMR Spectra of 1,6-Anhydro-2,3-Dideoxy-2,3-Epimino- and 1,6-Anhydro-3,4-Dideoxy-3,4-Epimino-ß-D-Hexopyranoses. Collect. Czech. Chem. Commun. 66(5), 799-819 (2001).
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5. Schraml J., Blechta V., Soukupová L., Petráková E.: DOSY of Silylated Saccharides. J. Carbohydr. Chem. 20(1), 87-91 (2001).
6. Bártlová M., Opletal L., Chobot V., Sovová H.: HPLC Analysis of Supercritical Carbon Dioxide Extracts of Schizandra chinensis. J. Chromatogr., B, submitted.
7. Herlin-Boime N., Ténégal F., Bastl Z., Šubrt J., Jursíková K., Blechta V., Pola J.: IR Laser Thermolytic Conversion of Disiloxanes to Polyoxocarbosilane Phase and Silicon Carbide. J. Mater. Chem., submitted.
8. Ossor A., De Bruyn A., Schraml J., Herdewijn P., De Keukeleire D.: A Novel Polyhydroxylated Alkaloidal Amine from Solanum elaeagnifolium with Beta-Glucosidase- and Neuraminidase Inhibiting Activity. FEBS Lett., submitted.
9. Pekárek V., Karban J., Fišerová E., Bureš M., Pacáková V., Večerníková E.: Why the Fly Ash Acts as the Dehalogenating Agent? Environ. Sci. Technol., submitted.
10. Podlaha J., Císařová I., Kvíčalová M., Schraml J.: Self-Assembly of 4-Nitrobenz-hydroxamic Acid in the Crystal. Supramol. Chem., submitted.
11. Pola J., Kupčík J., Blechta V., Galíková A., Galík A., Šubrt J., Kurjata J., Chojnowski J.: Thermally Stable Polyoxocarbosilane Thin Films by IR Laser Ablation of Poly[oxy(tetramethyldisilanediyl)]. Chem. Mater., in press.

Review papers

12. Schraml J., Soukupová L., Blechta V., Karban J., Císařová I.: Structure of Monosilylated Benzhydroxamic Acids in Crystals and Solutions. 628, 81-90 (2001).

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13. Schraml J.: ^{29}Si NMR Experiments in Solutions of Organosilicon Compounds. In: The Chemistry of Organic Silicon Compounds. Volume 3. (Rappoport, Z., Apeloig, Y., Eds.), pp. 223-339, J. Wiley, Chichester 2001.

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14. Auerová K., Čermák Jan, Nguyen H.T.T., Blechta V.: The Synthesis of Rhodium Complexes with Cyclopentadienyl Ligands Containing Perfluoroalkyl Ponytails. 3rd International School of Organometallic Chemistry, Abstracts, pp. 39-40, Camerino, Italy, 09-13 September 2001.
15. Bártlová M., Opletal L., Chobot V., Sovová H.: HPLC Analysis of Supercritical CO_2 Extracts of Schizandra chinensis. 2nd International Symposium Separations in the BioSciences SBS 2001, Book of Abstracts, p. 64, Prague, Czech Republic, 17-20 September 2001.
16. Čermák Jan, Kvíčalová M., Auerová K., Blechta V., Vojtíšek P., Kvíčala J.: Pentamethylcyclopentadienyl Metal Complexes: from Supported Catalysts to Biphase Systems. 10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Book of Abstracts, p. 38, Lyon, France, 02-06 July 2001.
17. Jochová M., Horáček J., Punčochář M.: Cleaning of Underground Water by Coal Based Sorbents. 28th International Conference of Slovak Society of Chemical Engineering, Book of Abstracts, p. 89, Tatranské Matliare, Slovakia, 21-25 May 2001.

Miscellaneous

International Advisory Board of ICPF

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Organization of International Conferences and Scientific Meetings

Scientific Meeting of COST F2 "Electrochemical Sensors for Flow Diagnostics", Vila Lanna, Prague, 03-06 May 2001

Scientific Meeting of INCO-Copernicus "Novel Techniques for Industrial Implementation of Immobilized Biocatalysts", ICPF, Prague 29-31 May 2001

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I. Wichterle: "Chemical Engineering and Technology"
R. Ponec: "Advances in Molecular Similarity (JAI Press)"
J. Drahoš: "International Journal of Multiphase Flow"
J. Drahoš: "Clean Products and Processes"
J. Hetflejš: "Chemické listy"