

Academy of Sciences of the Czech Republic

**Institute of Chemical Process  
Fundamentals of the ASCR, v. v. i.**

**Praha**

ANNUAL REPORT 2008

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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 serves 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, biochemical, environmental engineering and processes, physical chemistry, organic chemistry, industrial chemistry, and biotechnology.

## MANAGEMENT

Director	Jiří Hanika
Deputy Director (Research)	Jiří Smolík
Deputy Director (Business Administration) (since July 2008)	Eva Melková Olga Šolcová
Scientific Secretary	Jan Linek
Chairman of the Institute Board	Karel Aim

## DEPARTMENTS

Department of Separation Processes (page 6)  
E. Hála Laboratory of Thermodynamics (page 17)  
Department of Catalysis and Reaction Engineering (page 27)  
Department of Multiphase Reactors (page 39)  
Department of New Processes in Chemistry and Biotechnology (page 48)  
Environmental Process Engineering Laboratory (page 53)  
Laboratory of Aerosol Chemistry and Physics (page 62)  
Laboratory of Laser Chemistry (page 70)  
Department of Analytical Chemistry (page 74)

**STAFF**

(31 December 2008)

Category	Number of Employees
Research	140
Technical	20
Administrative	14
Services	15

**BUDGET 2008**

(17 Kč ≈ 1 US\$, 25 Kč ≈ 1 EUR)

Resources	Million Kč
Institutional support based on Institutional Research Plan	112
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	42
Foreign R&D Funds and European Programmes	7
Contracts with industry	5
<b>Total Resources</b>	<b>166</b>

Expenses	Per cent of Total Resources
Personal expenses including mandatory insurance	53
Purchase of material	8
Purchase of services	8
Repairs and maintenance	2
Depreciation of fixed assets	20
Travel expenses	3
Energy, water, and fuels	3
<b>Total other expenses</b>	<b>3</b>

## Abbreviations used throughout the Report

ASCR	Academy of Sciences of the Czech Republic
CTU	Czech Technical University, Prague
CU	Charles University, Prague
GA CR	Grant Agency of the Czech Republic
ICPF	Institute of Chemical Process Fundamentals of the ASCR, v. v. i., Prague
ICT	Institute of Chemical Technology, Prague
IIC	Institute of Inorganic Chemistry of the ASCR, v. v. i., Prague
IMC	Institute of Macromolecular Chemistry of the ASCR, v. v. i., Prague
IOCB	Institute of Organic Chemistry and Biochemistry of the ASCR, v. v. i., Prague
JH IPC	J. Heyrovský Institute of Physical Chemistry of the ASCR, v. v. i., Prague
MEYS	Ministry of Education, Youth and Sport of the Czech Republic
MIT	Ministry of Industry and Trade of the Czech Republic
TU	Technical University
UJEP	Jan Evangelista Purkyně University, Ústí n/L.
UPa	University of Pardubice

## Department of Separation Processes

Head: V. Jiříčný  
Deputy: A. Heyberger  
Research staff: J. Hanika, L. Hanková, L. Holub, P. Izák, K. Jeřábek, M. Kohoutová, J. Křišťál, R. Petříčkovič, K. Rochová, M. Rousková, J. Řezníčková, M. Sajfrtová, K. Setníčková, K. Soukupová, H. Sovová, P. Stavárek, P. Uchytíl  
Part time: V. Staněk, Z. Vajglová, M. Veselý, E. Volaufová, H. Vychodilová, P. Zálaha  
Technical staff: A. Kadlecová, D. Karfík, M. Koptová, D. Vlček  
PhD students: M. Poloncarzová

### Fields of research

- Research and development of electrochemical bipolar microreactor for electrochemical alkoxylation process
- Hydrodynamics of two phase flow in narrow channel
- Liquid extraction of tall oil from wastewaters of paper industry
- Fluorinated hydrocarbons as potential solvents in liquid extraction processes
- Supercritical fluid extraction of biologically active substances
- Enzymatic reactions in supercritical CO<sub>2</sub>
- Relation between the morphology and application properties of polymer catalysts and adsorbents
- Study of mass transport during vapour permeation and pervaporation in polymeric membranes
- Study of vapour condensation effect in ceramic membranes pores
- Separation of racemic mixtures
- Separation of gasoline vapours from air by supported ionic liquids membranes

### Applied research

- Extraction of polyaromatic hydrocarbons from aromatic petroleum fraction (300–400 °C)
- Extraction and production of plastic modifiers for production of tyres
- Extraction and refining of plant extracts
- Liquid extraction of luminophores, recycling of Y and Eu
- Applications of ion exchangers as catalysts in various industrial processes

## Research projects

### **Integrated multiscale process units with locally structured elements (IMPULSE)**

(J. Hanika, V. Jiříčný, J. Drahoš, 6th FP integrated project, Priority 3 NMP, supported by EU under Contract No. 011816-2)

The objective of IMPULSE project is effective, targeted integration of innovative process equipment such as microreactors, heat exchangers, thin-film devices and other micro components to attain radical performance enhancement for whole process systems in chemical production. We are involved in the application research of electroorganic synthesis in electrochemical microreactor. Extensive experimental research and development of electrochemical bipolar microreactor has been studied and applied on electrochemical alkoxylation process. The results of this research are a part of the research in several subtasks of the project. [Refs. 10, 41, 58]

### **Oxidation reactions and reactors for processing of raw material from renewable sources**

(V. Jiříčný, supported by ICPF)

The capillary microreactor has been utilized for Fenton oxidation of glycerol. The higher conversion has been reached in comparison with packed reactor under comparable conditions. The promising results from these preliminary experiments will be completed in the frame of new project submitted to GA CR.

### **Reclaiming of phytosterols and other valuable compounds from tall soap/oil**

(A. Heyberger, joint project with Technological Park Chomutov and Institute of Systems Biology and Ecology of the ASCR, v.v.i., supported by ASCR, project No. 1QS400720504)

The aim of the project is to study the tall soap composition and to develop methods of extractive separation of the valuable compounds. Besides of working out the necessary analytical methods, the extraction equilibria in systems with various solvents are measured, and the separation processes will be simulated in a laboratory vibrating plate extraction column. A novel extraction processes and equipment will be designed for recovering phytosterols and unsaturated fatty acids from tall soap. [Refs. 29, 37, 48, 49]

### **Two challenges of supercritical processes: flow pattern in extractor/reactor and fractionation of outflowing mixture**

(H. Sovová, supported by GACR, grant No. GA104/06/1174)

Axial mixing in a packed-bed extractor was examined using the tracer-response method [Refs. 46, 47]. Different ways how to affect the composition of a mixture of substances extracted with supercritical CO<sub>2</sub> from a plant were tested: use of entrainers for mixtures of substances of different polarity [Ref. 17] use of milder conditions to decrease the solubility of substances in CO<sub>2</sub> and thus increase the selectivity [Refs. 50, 56] and affect fatty acid composition of vegetable oil extracted from seeds by regiospecific enzymatic hydrolysis of the oil dissolved in supercritical CO<sub>2</sub> [Refs. 3, 16, 18, 55].

### **Supramolecular materials based on natural phytosterols for applications in biology**

(H. Sovová, joint project with IOCB, ICT, and Chemispol, supported by MEYS, project No. 2B06024)

The aim of the project is to utilise plants as a source of sterols representing starting stock for synthesis of supramolecules. The part of the project solved in the ICPF concerns supercritical fluid extraction of phytosterols and phytoecdysteriods from different plants rich in these substances. The extraction of 20-hydroxyecdysone from the leaves and root of

*Leuzea carthamoides* was studied in detail [Ref. 17]. Extraction condition-dependent separation factors of beta-sitosterol to major components in extracts from seed, leaf and pulp of sea buckthorn were evaluated [Refs. 50, 56].

### **Optimization of supercritical fluid extraction for maximal yield of biologically active substances from plants**

(H. Sovová, joint project with Research Institute of Plant Production and Agra Group, supported by MEYS, project No. 2B06049)

Essential oils and oleoresins were isolated from different plants using supercritical extraction hydrodistillation, and Soxhlet extraction and the effect of applied separation methods on insecticidal activity of isolates was determined [Refs. 51, 52]. Out of more than 20 examined plants, the isolates of *Satureja hortensis* showed a high activity against several model insects [Ref.11]. Besides, the literature on thin layer chromatography of lignans, efficient insecticides, was reviewed [Ref. 27].

### **Determination of biological activity and chemical composition of selected tropical and subtropical Ranunculaceae species**

(H. Sovová, joint project with Czech University of Life Sciences, and IOCB, supported by GACR, grant No. GA525/08/1179)

Essential oil of *Nigella sativa* contains biologically active substances thymoquinone and thymohydroquinone. The effect of pressure, temperature and solvent modifiers on the content of both substances in supercritical CO<sub>2</sub> extracts was examined. [Refs. 9, 42]

### **Synthesis, nanometer scale characterization and reactivity of metal (0)/macroreticular resin nanocomposites**

(K. Jeřábek, joint project with Istituto di Scienze e Tecnologie Molecolari, C. N. R., Sezione di Padova c/o Dipartimento di Chimica Inorganica Metallorganica Analitica, Padua, Italy, supported in the framework of the cooperation of ASCR and CNR, Italy)

The project is connected with our long-time research of morphology of swollen functional polymers in cooperation with Italian colleagues from Padua University, Italy. We studied the metal nanoparticle catalysts supported in polymer gel networks [Refs. 19, 21, 26].

### **Porosity investigations of PolyHIPEs using ISEC method**

(K. Jeřábek, joint project with University of Maribor, Slovenia, supported by MEYS, KONTAKT project No. MEB 090811)

The project combines Slovenian experiences with preparation of special functional polymers of PolyHIPE type with Czech skill in characterization of the morphology of polymer materials in their working that is swollen state. [Ref. 7]

### **Metal nanoparticles generated in polymer supports**

(K. Jeřábek, supported by ICPF)

Pilot samples were prepared of novel palladium nanoparticle catalysts supported using a proprietary process inside polymer matrix of commercial styrene-co-divinylbenzene polymers. Their practical tests performed by an industrial partner shown quite promising results.



### **Ceramic materials with hierarchical porous structure for membrane separation technologies**

(P. Uchytíl, joint project with ICT, JH IPC, and UPa, supported by ASCR, project No. 1QS401250509)

The adsorption experiments of pure gases and their mixtures on Vycor glass membranes with the group of Prof. Andreas Seidel-Morgenstern (Otto von Guericke University of Magdeburg, Max-Planck Institute, Magdeburg) were performed to study the mechanism of gas transport in these materials. For multicomponent systems, the description of adsorption equilibria can be quite difficult. It is often most convenient if adsorption equilibria are represented by explicit equations. In most cases two or three parameters which already appear in the single isotherms are preferred as realistic and theoretically valid. In this paper the Langmuir isotherm, the most popular two-parameter isotherm, was extended with corrections based on statistical solution as one way of data representation. [Refs. 14, 61]

### **Mass transport during membrane permeation and pervaporation**

(P. Uchytíl, joint project with University of Colorado, Boulder, USA, supported by MEYS, KONTAKT project No. ME 889)

Apparatus for simultaneous measurements of solubility, diffusivity and permeability of vapors in polymer film during a single experiment was designed. The main advantage of this sweeping-gas apparatus with a new type of a permeation cell is the possibility to determine an amount of permeates sorbed in the membrane in a steady state of a vapor permeation process without a need of any manipulation with the membrane. Data on permeate sorption in the membrane provide important information about transport mechanism in polymeric membranes. [Ref. 53]

### **Pervaporation and nanofiltration with ionic liquids**

(P. Izák, supported by EU Marie Curie Reintegration project No. MERG-CT-2006-044737)

The pervaporation proved to be one of the best methods to remove solvents out of a solvent producing *Clostridium acetobutylicum* culture. By using an ionic liquid – polydimethylsiloxane ultrafiltration membrane, we could guarantee high stability and selectivity (enrichment factor of butan-1-ol reached 11.23 at 3.75 g/l of its concentration in culture vessel) during all measurements carried out at 37 °C. By pervaporation through supported ionic liquid membrane we removed more butan-1-ol than *Clostridium acetobutylicum* was able to produce. Therefore we added an extra dose of butan-1-ol to run fermentation on limiting values, where the bacteria would still be able to survive. After the pervaporation was switched off, the bacteria died from high concentration of butan-1-ol, which they produced. [Refs. 6, 40]

### **Ionic membranes for selective separation of liquid mixtures by pervaporation**

(P. Izák, joint project with ICT, supported by GA CR, grant No. GA104/08/0600)

Ionic liquids seem to have a large potential in downstream processing, especially when applied in a form that requires only a small amount of them, e.g. in supported liquid membranes. The special property of ILs is their non-measurable vapor pressure that makes their application in liquid membranes attractive for pervaporation. The objective is to investigate the development and application of supported liquid membranes on the base of ionic liquids. The project will be focused on products of biotransformation, waste water treatment and other valuable products, where practical application in industry is ensured. [Refs. 22, 43]

## International co-operations

- ÅBO Akademi Process Chemistry Centre, Finland: By-product in the technology of sulfate cellulose production
- CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials
- University of KwaZulu-Natal, Republic of South Africa: Liquid-liquid extraction processes
- Institute of Chemical Engineering, Sofia, Bulgarian AS: High-pressure phase equilibria
- Institut National Polytechnique de Lorraine, Nancy, France: Research of electroorganic synthesis in electrochemical micro reactor
- Institute of Macromolecules, St. Petersburg, Russian Academy of Science, Russia: Membrane separation
- Institute für Mikrotechnik Mainz, Mainz, Germany: Research and development of micro devices
- Otto von Guericke University of Magdeburg, Magdeburg, Germany: Mass transport through porous membranes
- Solvent Innovation GmbH, Köln, Germany: Research of electroorganic synthesis in electrochemical micro reactor
- Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapors through porous membranes
- University of Barcelona, Barcelona, Spain: Morphology of polymer catalysts
- University of Linz, Linz, Austria: Determination of organic pollutants in water
- University of Padua, Padua and University of L'Aquila, L'Aquila, Italy: Molecular accessibility of microporous matrixes
- Nankai University, Tianjin, China: Hypercrosslinked polymer adsorbents
- University of Maribor, Maribor, Slovenia: Morphology of functional polymers
- Technical University of Lisbon, Portugal: Supercritical extraction of biological compounds from aromatic plants
- University of Colorado, Boulder, USA: Mass transport during vapour permeation and pervaporation, ionic liquids

## Visits abroad

- A. Heyberger: CSIR of Johannesburg, University of KwaZulu-Natal, Durban, South Africa (1 month)
- J. Křišťál: Procter & Gamble, Brussels, Belgium (8 months)
- P. Stavárek: CNRS Lyon, France (8 months)

## Visitors

- M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
- D. Ramjugernath, University of KwaZulu-Natal, Durban, Republic of South Africa
- J. Dudas, CSIR, Johannesburg, Republic of South Africa

## Teaching

J. Hanika: ICT, course and postgradual course "Multiphase reactors"

J. Hanika: ICT, course "Pharmaceutical engineering"

J. Hanika: UPa, course "Industrial catalysis"

H. Sovová: ICT, postgraduate course "Properties and application of supercritical fluids"

## Publications

### Original papers

1. Akramov T.A., Stavárek P., Jiříčný V., Staněk V.: Analysis of the Conditions for the Inception of Natural Pulsing Flow in Cocurrent Packed Columns. *Ind. Eng. Chem. Res.* 47(19), 7424-7432 (2008).
2. Hanika J.: Festina Lente. (Czech) More Haste. *Chem. Listy* 102(11), 955-956 (2008).
3. Hlavsová K., Wimmer Z., Xanthakis E., Bernášek P., Sovová H., Zarevúcka M.: Lipase Activity Enhancement by SC-CO<sub>2</sub> Treatment. *Z. Naturforsch. B* 63b(6), 779-784 (2008).
4. Izák P., Godinho M.H., Brogueira P., Figueirinhas J.L., Crespo J.G.: 3D Topography Design of Membranes for Enhanced Mass Transport. *J. Membr. Sci.* 321(2), 337-343 (2008).
5. Izák P., Ruth W., Fei Z., Dyson J.P., Kragl U.: Selective Removal of Acetone and Butan-1-ol from Water with Supported Ionic Liquid-Polydimethylsiloxane Membrane by Pervaporation. *Chem. Eng. J.* 139(2), 318-321 (2008).
6. Izák P., Schwarz K., Ruth W., Bahl H., Kragl U.: Increased Productivity of *Clostridium Acetobutylicum* Fermentation of Acetone, Butanol, and Ethanol by Pervaporation through Supported Ionic Liquid Membrane. *App. Microbiol. Biotechnol.* 78(4), 597-602 (2008).
7. Jeřábek K., Pulko I., Soukupová K., Štefanec D., Krajnc P.: Porogenic Solvents Influence on Morphology of 4-Vinylbenzyl Chloride Based polyHIPEs. *Macromolecules* 41(10), 3543-3546 (2008).
8. Jezerská L., Bělohav Z., Durdil P., Hanika J., Jašprová D., Tomášek V., Zámotný P.: Výzkum a modelování přímého lisování a vlhké granulace. (Czech) Research and Modeling of Direct Compaction and Wet Granulation. *Česká a slovenská farmacie* 57(1), 43 (2008).
9. Kokoška L., Havlík J., Valterová I., Sovová H., Sajfrtová M., Jankovská I.: Comparison of Chemical Composition and Antibacterial Activity of *Nigella sativa* Seed Essential Oils Obtained by Different Extraction Methods. *J. Food Prot.* 71(12), 2475-2480 (2008).
10. Kříšťál J., Kodým R., Bouzek K., Jiříčný V.: Electrochemical Microreactor and Gas-Evolving Reactions. *Electrochem. Commun.* 10(2), 204-207 (2008).
11. Pavela R., Sajfrtová M., Sovová H., Bárnét M.: The Insecticidal Activity of *Satureja hortensis* L. Extracts Obtained by Supercritical Fluid Extraction and Traditional Extraction Techniques. *Jpn. J. Appl. Entomol. Zool.* 43(3), 377-382 (2008).
12. Randová A., Hovorka Š., Izák P., Bartovská L.: Swelling of Nafion in Methanol-Water-Inorganic Salt Ternary Mixtures. *J. Electroanal. Chem.* 616, 117-121 (2008).
13. Rochová K., Sovová H., Sobolík V., Allaf K.: Impact of Seed Structure Modification on the Rate of Supercritical CO<sub>2</sub> Extraction. *J. Supercrit. Fluids* 44(2), 211-218 (2008).

14. Řezníčková Čermáková J., Marković A., Uchytíl P., Seidel-Morgenstern A.: Single Component and Competitive Adsorption of Propane, Carbon Dioxide and Butane on Vycor Glass. *Chem. Eng. Sci.* 63(6), 1586-1601 (2008).
15. Skála D., Hanika J.: Dicyclopentadiene Hydrogenation in Trickle Bed Reactor under Forced Periodic Control. *Chem. Pap.* 62(2), 215-218 (2008).
16. Sovová H., Lísa M., Holčápek M.: Estimation of Stereospecific Fatty Acid Distribution in Vegetable Oils from Liquid Chromatography Data A. *Eur. J. Lipid Technol.* 110(3), 266-276 (2008).
17. Sovová H., Opletal L., Sajfrtová M., Bártlová M.: Supercritical Fluid Extraction of Cynaropicrin and 20-Hydroxyecdysone from *Leuzea carthamoides* DC. *J. Sep. Sci.* 31(8), 1387-1392 (2008).
18. Sovová H., Zarevúcka M., Bernášek P., Stamenič M.: Kinetics and Specificity of Lipozyme-Catalysed Oil Hydrolysis in Supercritical CO<sub>2</sub>. *Chem. Eng. Res. Des.* 86(7), 673-681 (2008).
19. Centomo P., Zecca M., Králik M., Gasparovičová D., Jeřábek K., Canton P., Corain B.: Cross-linked Poly-vinyl Polymers versus Polyureas as Designed Supports for Catalytically Active M0 Nanoclusters Part II. Pd0/Cross-linked Poly-vinyl Polymers versus Pd0/EnCatTM30NP in Mild Hydrogenation Reactions. *J. Mol. Catal. A-Chem.* 300(1-2), 48-58 (2009).
20. Dudas J., Hanika J.: Design, Scale up and Safe Piloting of Thymol Hydrogenation and Menthol Racemisation. *Chem. Eng. Res. Des.* 87(1), 83-90 (2009).
21. Centomo P., Zecca M., Zoleo A., Maniero A.L., Treacher K., Canton P., Jeřábek K., Corain B.: Cross-linked Poly-vinyl Polymers versus Polyureas as Designed Supports for Catalytically Active M0 Nanoclusters. Part II. Nanometer Scale Structure of the Polyurea Support EnCat 30, of the Macromolecular Complex PdII/EnCat 30 and of the Catalyst Pd0/EnCat 30NP. *Macromolecules*, in press.
22. Izák P., Friess K., Hynek V., Ruth W., Fei Z., Dyson J.P., Kragl U.: Separation Properties of Supported Ionic Liquid-Polydimethylsiloxane Membrane in Pervaporation Process. *Desalination*, in press.
23. Petričkovič R., Setničková K., Uchytíl P.: New Apparatus for Gas Permeability, Diffusivity and Solubility Assessing in Dense Polymeric Membranes. *J. Membr. Sci.*, submitted.
24. Procházka J., Heyberger A., Volaufová E.: Effect of Diluents on Sulfuric Acid Extraction with Trialkylamine. *AIChE J.*, submitted.
25. Randová A., Bartovská L., Hovorka Š., Poloncarzová M., Kolská Z., Izák P.: Application of the Group Contribution Approach to Nafion Swelling. *J. Appl. Polym. Sci.*, in press.
26. Soukupová K., Sassi A., Jeřábek K.: Reinforcing of Expanded Polymer Morphology Using Peroxy Radical Initiator. *React. Funct. Polym.*, submitted.

#### Chapters in books

27. Opletal L., Sovová H.: TLC of Lignans. In: *Thin Layer Chromatography in Phytochemistry.* (Waksmundzka-Hajnos, M. - Sherma, J. - Kowalska, T., Ed.), pp. 425-449, CRC Press, New York 2008.
28. Warshawsky A., Cortina J.L., Jeřábek K.: Solvent Impregnated Resins Applications on Metal Separation Processes. In: *Solvent Extraction and Liquid Membranes.* (Aguilar, M. - Cortina, J.L., Ed.), pp. 301-334, CRC Press, New York 2008.

## Patents

29. Heyberger A., Tříska J., Rousková M., Krtička M.: Způsob a zařízení k získávání fytosterolů. (Czech) Process and Equipment for Phytosterols Recovering. Pat. No. PV 2008-852. Applied: 08.12.30.
30. Novák L., Černín A., Hanika J., Veselý V.: Způsob a zařízení pro izolaci kyseliny tereftalové. (Czech) Princip and Device for Terephthalic Acid Isolation. Pat. No. PV 2008-602. Applied: 08.10.09.

## International conferences

31. Banavali R., Hanlon R.T., Jeřábek K., Schultz A.K.: Heterogeneous Catalyst and Process for the Production of Biodiesel from High Free-Fatty Acid-Containing Feedstocks. 22nd Biennial ORCS Conference on the Catalysis of Organic Reactions, Richmond, Virginia, USA, 30 March - 03 April 2008.
32. Bártová D., Jakeš B., Jiříčný V., Kukul J., Staněk V., Stavárek P.: Study of Dispersion Flow in Trickle Bed Reactor. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 868 (11 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
33. Gogová Z., Hanika J.: Model Aided Design of Gas-Lift Reactor for Oxidation Reaction with Fast Reversible Catalyst Deactivation. 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, Book of Abstracts p. 711 (6 pp. full text on CD-ROM), Braga, Portugal, 04-06 September 2008.
34. Gogová Z., Hanika J.: Design of Gas-Lift Reactor for Catalytic Oxidation. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 1, p. 248, Praha, Czech Republic, 24-28 August 2008.
35. Gogová Z., Hanika J.: Purpose Tailored Design of Gas-Lift Reactor. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 271 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
36. Hanková L., Corain B., Jeřábek K.: Swollen State Morphology of Novel Polyurea-supported EnCat Catalysts. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 160 (6 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
37. Heyberger A., Tříska J., Rousková M., Růžicková K., Volaufová E., Krtička M.: Tall Soap Liquid-Liquid Extraction - Study of the Different Parameters during the Process and Their Influence to the Extract Composition. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 378 (5 pp. full text on CD-ROM), Praha, Czech Republic, 25-28 August 2008.
38. Izák P., Godinho M.H., Brogueira P., Figueirinhas J.L., Crespo J.G.: Surface Modification of Pervaporation Membrane by UV-Radiation and Application of Shear Stress. International Congress on Membranes and Membrane Processes, Oral Presentation Proceedings, Honolulu, Hawaii, USA, 12-18 July 2008.
39. Izák P., Mateus N.M.M., Afonso C.A.M., Crespo J.G.: Enhanced Esterification Conversion in a Room Temperature Ionic Liquid by Integrated Water Removal with Pervaporation. 9th Pannonian International Symposium On Catalysis, Book of Abstracts, pp. 1-6, Štrbské Pleso, Slovakia, 08-12 September 2008.
40. Izák P., Schwarz K., Kohoutová M., Ruth W., Bahl H., Kragl U.: Fermentation Coupled with Pervaporation. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 54 (13 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.

41. Křišťál J., Havlica J., Jiříčný V.: Hydrodynamic Characterization of Electrochemical Microreactor. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 5, p. 1726 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
42. Malík J., Sajfrtová M.S., Kokoška L.: Antioxidative Potential of Root Extracts from Certain Ranunculaceae Species. 1st European Food Congress, Delegate Manual, p. P041, Ljubljana, Slovenia, 04-09 October 2008.
43. Randová A., Bartovská L., Hovorka Š., Izák P., Poloncarzová M., Kolská Z.: Swelling of Nafion Membrane Predicted by the Group Contribution Method. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 607 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
44. Randová A., Bartovská L., Izák P., Hovorka Š., Friess K.: Sorption of Liquid Mixture Methanol – Benzene in Polymeric Membranes. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 624 (5 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
45. Randová A., Izák P., Hovorka Š., Bartovská L.: Separation Properties of Nafion and LDPE Membrane. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 333 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
46. Rochová K., Sovová H.: Flow Pattern in a Packed Bed Supercritical Extractor. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 537 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
47. Rochová K., Sovová H.: Flow Pattern in a Packed Bed Supercritical Extractor. 11th European Meeting on Supercritical Fluids, Abstracts, p. 316, Barcelona, Spain, 04-07 May 2008.
48. Rousková M., Heyberger A., Tříška J.: Problematika extračního zpracování tálového mýdla. (Czech) Problems in Extraction Processing of Tall Soap. 17. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, p. 1312-1327, Milovy, Czech Republic, 14-16 April 2008.
49. Rousková M., Volaufová E., Heyberger A., Tříška J., Krtička M.: Influence of pH and Deemulsifier of Extraction Refining of Tall Soap Components. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 176 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
50. Sajfrtová M., Sovová H., Bártlová M.: Supercritical Fluid Extraction of beta-Sitosterol from Sea Buckthorn Pulp and Leaves. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 542 (6 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
51. Sajfrtová M., Sovová H., Karban J., Pavela R.: Insecticide Activity of Herb Extracts Isolated by Different Methods. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 541 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
52. Sajfrtová M., Sovová H., Pavela R.: Effect of Extraction Methods on Botanical Insecticide Activity. 11th European Meeting on Supercritical Fluids, Abstracts, p. 282, Barcelona, Spain, 04-07 May 2008.
53. Setničková K., Petříčkovič R., Uchytíl P.: Importance of Steady State Sorption Data for Vapor Permeation Transport Description and Their Measurements. International Congress on Membranes and Membrane Processes, Poster Session Proceedings, pp. 89-90, Honolulu, Hawaii, USA, 12-18 July 2008.

54. Smejkal Q., Kolena J., Hanika J.: Ethyl Acetate Synthesis by Coupling of Fixed Bed Reactor and Reactive Distillation Column - Process Integration Aspects. XVIII International Conference on Chemical Reactors CHEMREACTOR-18, Scientific Program, p. 20 (pp. 112-114 full text on CD-ROM), Malta, Malta, 29 September - 03 October 2008.
55. Sovová H., Rochová K., Sajfrtová M.: Oil Processing with SC-CO<sub>2</sub>: From Seed to Reaction Products. 11th European Meeting on Supercritical Fluids, Abstracts, p. 97, Barcelona, Spain, 04-07 May 2008.
56. Sovová H., Sajfrtová M., Rochová K.: Plant Extracts as Mixtures and Their Prefractionation by Supercritical CO<sub>2</sub>. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 343 (10 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
57. Stavárek P., Staněk V., Jiříčný V.: Comparison of Tracer and Weighting Method for Liquid Holdup Measurement in the Trickle Bed Reactor. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 1, p. 313 (6 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
58. Steckenborn A., Křišťál J., Kareš T., Jiříčný V., Sichler P., Krause P.: New Pressure Sensor for Applications in Micro Chemical Engineering. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 5, p. 1734 (9 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
59. Tukač V., Handlová M., Chyba V., Lederer J., Kolena J., Kubička D., Hanika J., Jiříčný V., Stavárek P.: Intensification of Pyrolysis Gasoline Hydrogenation in Pilot Trickle-Bed Reactor with Periodic Modulated Feed Rate. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 1, pp. 71-72 (10 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
60. Tukač V., Hanika J., Veselý V., Lederer J., Nečesaný V.: Termodynamický rozbor parciální oxidace bioodpadu a rafinerských zbytků. (Czech) Thermodynamics of Biowaste and Refinery Waste Partial Oxidation. 17. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, pp. 1174-1181, Milovy, Czech Republic, 14-16 April 2008.
61. Uchytíl P., Petříčkovič R.: Influence of Capillary Condensation Effect on Butane Transport through Porous Vycor Membrane. 10th International Conference on Inorganic Membranes, Program and Abstracts, p. 217, Tokyo, Japan, 18-22 August 2008.
62. Veselý V., Hanika J.: PET Bottles Recycling. Pollutec 2008, Workshop Proceedings, pp. 1-6, Lyon, France, 02-05 December 2008.
63. Veselý V., Hanika J., Čech B.: Nová metoda chemické recyklace PET lahví. (Czech) A New Method of PET Bottles Chemical Recycling. 60. Jubilejní sjezd asociací českých a slovenských chemických společností, Chemické Listy 102(8), p. 648, Olomouc, Czech Republic, 01-04 September 2008.
64. Wimmer Z., Sajfrtová M., Sovová H., Pavlík M., Svobodová H., Jurček O., Wimmerová M.: Alternativní využití rostlin pro získání významných přírodních látek: může najít využití i plevel? (Czech) Alternative Plant Utilization for Obtaining of Significant Nature Substances: Can Weed Find an Utilization? 14. odborný seminář s mezinárodní účastí: Aktuální otázky pěstování léčivých, aromatických a kořeninových rostlin, Sborník příspěvků, pp. 5-9, Lednice, Czech Republic, 02 December 2008.
65. Zámotný P., Bělohav Z., Durdil P., Hanika J., Jašprová D., Jezerská L., Tomášek V.: Effect of Mixture Properties and Mixing Parameters on Pharmaceutical Powder Homogenization. 18th International Congress of Chemical and Process Engineering

CHISA 2008, Summaries 5, p. 1745-1746 (9 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.



## E. Hála Laboratory of Thermodynamics

Head: K. Aim  
Deputy: M. Lísal  
Research staff: M. Bendová, J. Linek, L. Morávková, J. Pavlíček, Z. Sedláková, L. Vlček, Z. Wagner, I. Wichterle  
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Technical staff: S. Bernatová  
PhD students: J. Jirsák

### Fields of research

- Experimental determination and modelling of phase equilibria in fluid systems, including systems containing ionic liquids and systems with chemical reaction
- State and phase behaviour of fluids at superambient conditions (up to very high pressures)
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Molecular simulations of chemically reacting systems in nanoporous materials
- Mesoscale simulations of polymeric/nanoparticle systems
- Development of molecular theory of polar and associating compounds (and their mixtures)
- Development of equations of state based on molecular theory
- Development and application of density functional theory for inhomogeneous fluids
- Hydrophobic interactions
- Percolation and nucleation
- Application of statistical-mechanical models to real fluids
- Thermodynamic modelling and processing of thermodynamic data

### Applied research

- Computerized bibliography of vapour-liquid equilibrium data

### Research projects

#### **Determination of the phase and state behaviour of fluids and fluid mixtures for processes at superambient conditions: molecular-based theory and experiment**

(K. Aim, joint project with UJEP and CTU, supported by ASCR, grant No. IAA400720710)

Two new variants of the many-fluid density functional theory have been developed and their ability to describe orientational ordering in mixtures of model fluids of anisotropic hard

bodies has been assessed in detail. Molecular simulation studies were performed on the model fluid of hard spheres with a modified dipole and on Lennard-Jones mixtures to explain the effect of cross interactions on mixing properties. Research continued on applications of the perturbation theory using a reference system based on the short-range part of intermolecular interactions (which was shown to capture the main characteristic features of real fluids) to describe the thermodynamic behaviour of systems containing carbon dioxide + alkanols, for which experimental phase equilibrium data have been recently measured in our laboratory. [Refs. 2, 6, 12, 29, 30, 37, 38, 45]

### **Supercritical phase equilibria and p-V-T behaviour**

(M. Bendová, supported by GACR, grant No. GP104/06/P066)

A new apparatus for measurements of high-pressure phase equilibria by synthetic method was assembled, based on Thar Technologies Super Phase Monitor. The accuracy of the apparatus was first checked by measuring the solubilities of supercritical CO<sub>2</sub> and ethanol. Subsequently, solubilities of the supercritical CO<sub>2</sub> in the ionic liquid 1-ethyl-3-methylimidazolium ethylsulfate were measured. Experimental liquid-liquid equilibrium data acquired for binary systems of 1-ethyl-3-methylimidazolium ethylsulfate + heptane, or + methylcyclohexane, or + toluene and of 1-butyl-3-methylimidazolium hexafluorophosphate + water were thermodynamically described by a modified Flory-Huggins equation and molecular-thermodynamic lattice model proposed by Qin and Prausnitz. Liquid phase behaviour was studied in the quaternary system 1-butyl-3-methylimidazolium hexafluorophosphate + water + 1-chlorobutane + 1-methylimidazole [Refs. 1, 32, 33].

### **P-V-T behaviour of liquid mixtures modelling engine fuels – experimental determination, correlation and prediction**

(J. Linek, supported by GACR, grant No. GA104/06/0656)

Excess volumes at atmospheric pressure were determined in systems octane + benzene, or + toluene, or + 1,3-xylene, or + 1,3,5-trimethylbenzene at temperatures between 298.15 K and 328.15 K. Density, excess volume, and isothermal compressibility of octane + benzene system were measured and calculated along four isotherms between 298.15 K and 328.15 K at pressures up to 40 MPa. Novel fitting procedure developed by us for calculating the density and isothermal compressibility from Tait equation was applied. Densities and sound velocities were measured for binary systems composed of isooctane, toluene, and MTBE at four temperatures within 298.15 K and 328.15 K and atmospheric pressure. Statistic and gnostic methods were applied to fit the incomplete data of excess volumes. [Refs. 9, 10, 20, 39-41, 46]

### **Molecular simulations at extreme experimental conditions: Application of advanced methods to geochemistry**

(M. Lisal, supported by ASCR, project No. 1ET400720507)

New methods and algorithms for computer modelling and molecular simulations in geochemistry (particularly for geological fluid systems at extreme state conditions) have been developed. The main pursued lines of research were (i) state and phase behaviour of geological fluids at high temperatures and high pressures and (ii) physico-chemical properties of geological fluid systems in porous media. To this end, molecular simulation methodologies and density functional theory for non-reacting and high-density chemically-reacting fluid

systems both in the bulk and in confinement have been developed and tested. [Refs. 4, 23, 34, 42-44]

### **Design of “tailor made” multifunctional organic materials by molecular modelling of structure – property relationship, experimentation and processing (MULTIPRO)**

(M. Lísal, supported by FP6 RTD EU, project No. NMP3-CT-2006-033304)

The aim of MULTIPRO is to develop new multifunctional materials for opto-electronic devices based on solid state lighting sources, addressed to several applications (automotive head-up displays and lighting, public information displays and general lighting) and, at the same time, a new integrated reactive packaging technology suitable for the material developed and cost effective for the applications. MULTIPRO develops polymeric resins in which nanoparticles of different nature are built in or embedded in order to reach multifunctional material with new and improved properties. The specific material properties are controlled and tailored by changing nature, size, composition, and concentration of the nanoparticles according to industrial and technological request. MULTIPRO responds to the concept of the “tailor made”, which means that the above described functionalities respond to specific needs of a given application. Molecular modelling is the enabling technology to tailor the material in terms of components necessary for the properties desired. MULTIPRO also develops modelling procedures and dedicated software to simulate each step of materials development from the pure components structure to reactive models, up to the final materials, from which properties can be argued. [Refs. 7, 8, 35, 42, 52]

### **Computer modelling of structural, dynamical and transport properties of fluids in nanospace**

(M. Lísal, joint project with University of South Bohemia in Ceske Budejovice, supported by GACR, grant No. GA203/08/0094)

The aim of the new project is to study the behavior of fluids in the nanospace, solid-liquid interface (metal oxide-aqueous solution) and nanoporous carbons (activated carbons and carbon nanotubes) by equilibrium and nonequilibrium molecular simulations to provide structural, dynamical and transport properties of fluids in nanoconfinement. At solid-liquid interfaces, the simulation results for dynamics of water molecules are linked with quasielastic neutron scattering; the space-dependent shear viscosity and the dielectric properties are linked with electrophoretic data. We are also developing a method for the determination of local, space-dependent permittivity in inhomogeneous systems. In the case of nanoporous carbons, we adopt the methods for calculating local, space-dependent diffusivity and shear viscosity of pure fluids to slit and cylindrical nanopores, develop a method for the determination of space-dependent shear viscosity of fluid mixtures from computer simulations, and simulate the structural, dynamical and transport properties of industrially important fluid mixtures in carbon nanopores. [Refs. 4, 5, 19, 23, 24, 42-44, 53, 54]

### **Application of advanced simulation methods for studying the structure, physico-chemical properties, and preparation of composites and nanomaterials**

(I. Nezbeda, joint project with UJEP, supported by ASCR, project No. 1ET400720409)

A complex study was devoted to the treatment of long-range interactions in molecular simulations resulting in a set of recommendations [Ref. 2]. Another methodological study dealt with occurrence of an infinite cluster in finite size systems [Refs. 15, 59]. It was shown that the so called ‘wrapping’ cluster satisfies all physical constraints including universality. The effect of cross interactions on properties of mixtures was investigated by molecular simulations using model Lennard-Jones mixtures [Refs. 12, 55]. It was shown that deviations from the commonly used Lorentz-Berthelot rules may result even in qualitative changes in the behavior of mixtures. Within attempts to develop a molecular theory of fluids, extensive

simulation data were generated for a specific dipolar system for their use in a consequent research. [Further refs. 3, 18, 21, 36]

### **Simple and complex models of aqueous solutions: The effect of nonadditive interactions**

(I. Nezbeda, supported by ASCR, grant No. IAA4007720802)

Since the general goal of the new project is to develop a molecular theory of aqueous systems based on primitive models, systems of pseudo-hard bodies were studied both by simulations and theory. An analytic theory for their mixtures, based on the knowledge of a few virial coefficients, has been developed [Refs. 13, 47-50, 56].

### **Thermodynamic properties of gas-liquid systems**

(I. Wichterle, supported by GACR, grant No. GA104/07/0444)

Vapour-liquid equilibria in binary and ternary systems of species with selected functional groups (tert-butyl, isopropyl, carbonyl, ether, and hydroxyl) have been measured [Refs. 11, 17]. Liquid-liquid equilibrium data were determined in systems ionic liquid + water/alcohol/hydrocarbon [Refs. 1, 14, 32, 57, 58]. Phase equilibrium in system with transesterification reaction has been investigated [Ref. 29]. Algorithm was developed for reliable evaluation of temperature-independent parameters from vapour-liquid equilibria covering a temperature range [Refs. 22, 51]. The second volume of bibliographic database of VLE data has been published within the Landolt-Börnstein Encyclopaedia series [Ref. 26], concluding so the 35 years lasting project.

### **Novel technology of preparation of molecularly imprinted polymeric materials**

(I. Wichterle, supported by Ministry of Science, Education and Sports of Croatia, project No. MZOS-RH 061-0-3029)

Copolymers and terpolymers synthesized by polymerization of long chain methacrylates with styrene and (meth)acrylic acid with styrene or 1-vinyl-2-pyrrolidone are efficient flow improvers for oil transport. Liquid-vapour equilibria were determined by micro-ebulliometry for solutions of these polymers in toluene, hexane and chloroform at different temperatures and pressures. [Ref. 60]

### **EFCE Working Party "Fluid Separations"**

(M. Bendova, supported by MEYS, programme INGO project No. LA 320)

Activities connected with membership of M. Bendova in EFCE Working Party on "Fluid separations". Annual meeting of the WP was organized in Prague on 22-23 May, 2008.

## **International co-operations**

Technical University of Vienna, Austria: Colloids and theory of fluids

University of Ontario Institute of Technology, Oshawa, ON, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids

INA, Research and Development, Zagreb, Croatia: Properties of polymer solutions

ITODYS, University of Paris VII, France: Vapour-liquid equilibrium bibliographic database

Université de Paris-Sud, Orsay, France: Properties prediction of polymer systems using mesoscopic simulations based on dissipative particle dynamics method

Université François Rabelais, Tours, France: Liquid-liquid phase equilibria in systems of ionic liquids

University of Leipzig, Leipzig, Germany: Fluids at extreme conditions  
DICAMP, University of Trieste, Italy: Phase equilibria for supercritical fluid technology  
Universidad Rovira i Virgili, Tarragona, Spain: Molecular-based studies of chemically reacting systems in nanoporous materials  
Institute of Condensed Matter, Ukrainian Acad. Sci., Lviv, Ukraine: Modelling of molecular fluids at extreme conditions: Theory and applications  
Queen's University Ionic Liquids Laboratory (QUILL), Belfast, UK: Liquid-liquid phase equilibria in systems of ionic liquids  
U. S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale and molecular simulations of complex systems  
Oak Ridge National Laboratory, Oak Ridge, TN, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems

## Visits abroad

J. Jirsák: University of Ontario, Institute of Technology, Oshawa, ON, Canada (5 months)  
M. Lísal: University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)  
A. Malijevský: Imperial College, London, UK (12 months)  
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

## Visitors

B. Rousseau, Université de Paris Sud, Orsay, France  
K.M. Patterson, Pennsylvania State University, University Park, PA, USA  
A. Trokhymchuk, Institute of Condensed Matter Physics, Lviv, Ukraine  
R. Melnyk, Institute of Condensed Matter Physics, Lviv, Ukraine

## Teaching

M. Lísal: UJEP, courses "Parallel programming", "Numerical mathematics I" and "Numerical mathematics II"  
I. Nezbeda: UJEP, courses "Molecular simulations I", "Molecular theory of matter", "Kinetic theory" and "Principles of Scientific Communication"  
I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"  
M. Kotrla, M. Předota: CU, course "Advanced computer simulations in many particle systems"  
M. Předota: University of South Bohemia, Č. Budějovice, courses "Lectures from physics oriented to particle and nuclear physics" and "Selected lectures from physics"

## Publications

### Original papers

1. Bendová M., Wagner Z., Moučka M.: Liquid-Liquid Equilibrium in Binary System 1-Butyl-3-Methylimidazolium Hexafluorophosphate + Water. Experiment and Data Correlation. *Int. J. Thermodyn.* 11(3), 109-114 (2008).
2. Jirsák J., Nezbeda I.: Fluid of Hard Spheres with a Modified Dipole: Simulation and Theory. *Collect. Czech. Chem. Commun.* 73(4), 541-557 (2008).
3. Kolafa J., Moučka F., Nezbeda I.: Handling Electrostatic Interactions in Molecular Simulations: A Systematic Study. *Collect. Czech. Chem. Commun.* 73(4), 481-506 (2008).
4. Lísal M., Cosoli P., Smith W., Jain S.K., Gubbins K.E.: Molecular-level Simulations of Chemical Reaction Equilibrium for Nitric Oxide Dimerization Reaction in Disordered Nanoporous Carbons. *Fluid Phase Equilib.* 272(1-2), 18-31 (2008).
5. Machesky M.L., Předota M., Wesolowski D.J., Vlček L., Cummings P.T., Rosenqvist J., Ridley M.K., Kubicki J.D., Bandura A.V., Kumar N., Sofo J.O.: Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework. *Langmuir* 24(21), 12331-12339 (2008).
6. Malijevský A., Jackson G., Varga S.: Many-fluid Onsager density functional theories for orientational ordering in mixtures of anisotropic hard-body fluids. *J. Chem. Phys.* 129, 144504-1 - 144504-15 (2008).
7. Malý M., Posocco P., Fermeglia M., Pricl S.: Scripting Approach in Hybrid Organic-Inorganic Condensation Simulation: The GPTMS Proof-of-Concept. *Mol. Simul.* 34(10-15), 1215-1236 (2008).
8. Malý M., Posocco P., Pricl S., Fermeglia M.: Self-Assembly of Nanoparticle Mixtures in Diblock Copolymers: Multiscale Molecular Modeling. *Ind. Eng. Chem. Res.* 47(15), 5023-5038 (2008).
9. Morávková L., Linek J.: Excess Molar Volumes of (Octane + Benzene, or + Toluene, or + 1,3-Xylene, or 1,3,5-Trimethylbenzene) at Temperatures between (298.15 K and 328.15) K. *J. Chem. Thermodyn.* 40(4), 671-676 (2008).
10. Morávková L., Wagner Z., Linek J.: (p, Vm, T) Measurements of (Octane + Benzene) at Temperatures from (298.15 K to 328.15) K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.* 40(4), 607-617 (2008).
11. Psutka Š., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Propanol, 3-Methyl-2-butanone and 2,2,4-Trimethylpentane. *Fluid Phase Equilib.* 264(1-2), 55-61 (2008).
12. Rouha M., Moučka F., Nezbeda I.: The Effect of Cross Interactions on Mixing Properties: Non-Lorentz-Berthelot Lennard-Jones Mixtures. *Collect. Czech. Chem. Commun.* 73(4), 533-540 (2008).
13. Rouha M., Nezbeda I.: Thermodynamics of pseudo-hard body mixtures. *Mol. Phys.* 106, 2481-2485 (2008).
14. Sedláková Z., Sauton H., Hynek V., Malijevská I.: Solid-Liquid Equilibrium in the Systems with an Ionic Liquid. *Collect. Czech. Chem. Commun.* 73(5), 657-664 (2008).
15. Škvor J., Nezbeda I.: On Universality of the Wrapping Percolation Transition. *Collect. Czech. Chem. Commun.* 73(3), 401-412 (2008).
16. Ždímal V., Brabec M., Wagner Z.: Comparison of Two Approaches to Modeling Atmospheric Aerosol Particle Size Distributions. *Aerosol Air Quality Res.* 8(4), 392-410 (2008).

17. Bernatová S., Pavlíček J., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of tert-Butyl Methyl Ether, 3,3-Dimethyl-2-butanone and 2,2-Dimethyl-1-propanol. *Fluid Phase Equilib.*, submitted.
18. Maksimov M., Vlček L., Prokop A.: Development of Compartmental Tumor Uptake and Organ Washout Model for Drug and Imaging Purposes: Retrospective Study. *Mol. Pharmacol.*, submitted.
19. Mamontov E., Wesolowski D.J., Vlček L.: Dynamics of Hydration Water on Rutile Studied by Backscattering Neutron Spectroscopy. *J. Phys. Chem. C*, submitted.
20. Morávková L., Wagner Z., Linek J.: Volumetric Behaviour of Binary Liquid Systems Composed of Toluene, Isooctane and Methyl tert-Butyl Ether at Temperatures from 298.15 K to 328.15 K. *J. Chem. Thermodyn.*, in press.
21. Payne C.M., Zhao X., Vlček L., Cummings P.T.: Electrophoresis of Single-stranded DNA through Nanoelectrode Gaps from Molecular Dynamics: Impact of Gap Width. *Phys. Rev. E.*, submitted.
22. Wagner Z.: Robust Method of Determination of Interaction Parameters of Equation of State from High Pressure Vapour-Liquid Equilibrium Data. *Fluid Phase Equilib.*, submitted.

#### Review papers

23. Turner C.H., Brennan J.K., Lísal M., Smith W.R., Johnson J.K., Gubbins K.E.: Simulation of Chemical Reaction Equilibria by the Reaction Ensemble Monte Carlo Method: A Review. *Mol. Simul.* 34(2), 119-146 (2008).
24. Vlček L., Cummings P.T.: Adsorption of Water on TiO<sub>2</sub> and SnO<sub>2</sub> Surfaces: Molecular Dynamics Study. *Collect. Czech. Chem. Commun.* 73(4), 575-589 (2008).

#### Books and monographs

25. Linek J.: Annual Report 2007. 75pp., ICPF, Praha 2008.
26. Wichterle I., Linek J., Wagner Z., Fontaine J.-C., Sosnkowska-Kehiaian K., Kehiaian H.V.: Landolt-Börnstein IV/13A. Vapor-Liquid Equilibrium in Mixtures and Solutions. Part 2. 575 pp., 882 Figs., Springer, Berlin 2008. ISBN 978-3-540-70744-8.

#### International conferences

27. Ahlström P., Aim K., Dohrn R., Elliott R., Fele-Žilnik L., Jackson G., Jaubert J.-N., Macedo M.E.R., Pokki J.-P., Reczey K., Victorov A., Economou I.G.: A Survey of Thermodynamics and Transport Properties in Chemical Engineering Education in Europe and the USA. AICHE Annual Meeting 2008, Conference Proceedings, p. 148 (8 pp. full text on CD-ROM), Philadelphia, Pennsylvania, USA, 16-21 November 2008.
28. Aim K.: Central European Perspective: The Czech Scientific Model. AAAS Annual Meeting, Boston, USA, 15-18 February 2008.
29. Aim K., Nezbeda I.: Advances in the Description of Thermodynamic Properties of Alkanolic Systems. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, pp. 399-400 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
30. Aim K., Nezbeda I.: Thermodynamics and Phase Equilibria in Carbon Dioxide + Alkanol Systems from Statistical-Thermodynamics Theory. 23rd European Symposium on Applied Thermodynamics, Proceedings, p. 142, Cannes, France, 29 May - 01 June 2008.

31. Aim K., Wichterle I.: Reduction of Vapor-Liquid Equilibrium Data for System with Transesterification Reaction. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 411, Praha, Czech Republic, 24-28 August 2008.
32. Bendová M., Klusoň P., Sedláková Z., Wagner Z., Černá I., Vašinová J.: Liquid-Liquid Equilibrium in Quaternary System [bmim][PF<sub>6</sub>] + Water + 1-Methylimidazole + 1-Chlorobutane. 13th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Abstracts, Trinity College Dublin, Ireland, 28-31 July 2008.
33. Bendová M., Sedláková Z., Wagner Z.: Solubility of 1-Ethyl-3-methylimidazolium Ethylsulfate in Supercritical CO<sub>2</sub>. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 584, Praha, Czech Republic, 24-28 August 2008.
34. Brennan J.K., Lísal M., Bonet Avalos J.: Mesoscale Modeling of Energy Release Processes: Dissipative Particle Dynamics Simulations of Shear Initiated Behavior. AIChE Annual Meeting 2008, Conference Proceedings (4 pp. full text on CD-ROM), p. 716a, Philadelphia, PA, USA, 16-21 November 2008.
35. Fermeglia M., Pricl S., Posocco P., Malý M., Lísal M.: Computer Simulation of Hybrid Organic-Inorganic Nanocomposites. AIChE Annual Meeting 2008, Conference Proceedings (4 pp. full text on CD-ROM), p. 734c, Philadelphia, PA, USA, 16-21 November 2008.
36. Francová M., Maliževský A., Kolafa J., Labík S.: An Accurate Analytical Representation of the Bridge Function of Hard Spheres. 7th Liquid Matter Conference, Poster Presentations, p. PA:17, Lund, Sweden, 27 June - 01 July 2008.
37. Jirsák J., Nezbeda I.: Towards a Molecular Theory of Water. 7th Liquid Matter Conference, Poster Presentations, p. PB:21, Lund, Sweden, 27 June - 01 July 2008.
38. Jirsák J., Nezbeda I.: Towards a Molecular Theory of Water. 23rd European Symposium on Applied Thermodynamics, Proceedings, pp. 197-198 (4 pp. full text on CD-ROM), Cannes, France, 29 May - 01 June 2008.
39. Linek J., Morávková L., Wagner Z.: (p, V<sub>m</sub>, T) Measurements of (Octane + Benzene) at Temperatures from 298.15 K to 328.15 K and at Pressures up to 40 MPa. 23rd European Symposium on Applied Thermodynamics, Proceedings, p. 101 (4 pp. full text on CD-ROM), Cannes, France, 29 May - 01 June 2008.
40. Linek J., Morávková L., Wagner Z.: (p, V<sub>m</sub>, T) Measurements of (Octane + Benzene) at Temperatures from 298.15 K to 328.15 K and at Pressures up to 40 MPa. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 157 (4 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
41. Linek J., Morávková L., Wagner Z.: (P, V, T) Measurements of (Octane + Benzene) at Temperatures from 298.15 K to 328.15 K and at Pressures up to 40 MPa. 20th International Conference on Chemical Thermodynamics, Book of Abstracts, p. 295, Warsaw, Poland, 03-08 August 2008.
42. Lísal M., Brennan J.K.: Self-Assembly of Diblock Copolymers in Nanopatterned Confinement: Insight from Dissipative Particle Dynamics Simulations. AIChE Annual Meeting 2008, Conference Proceedings (4 pp. full text on CD-ROM), 470f, Philadelphia, PA, USA, 16-21 November 2008.
43. Lísal M., Cosoli P., Smith W.R., Jain S.K., Gubbins K.E., Aim K.: Molecular Simulations of Chemical Reaction Equilibrium for Nitric Oxide Dimerization Reaction in Disordered Nanoporous Carbons. 20th International Conference on Chemical Thermodynamics, Book of Abstracts, p. 267, Warsaw, Poland, 03-08 August 2008.



44. Malijevský A., Jackson G.: A Density Functional Study of Interfacial Properties of Spherical Fluid Interfaces. 7th Liquid Matter Conference, Poster Presentations, p. PG:60, Lund, Sweden, 27 June - 01 July 2008.
45. Malijevský A., Jackson G., Varga S.: Extension of Osanger Type Density Functional Theories for Hard Body Fluid Mixtures. 7th Liquid Matter Conference, Poster Presentations, p. PC:21, Lund, Sweden, 27 June - 01 July 2008.
46. Morávková L., Wagner Z., Linek J.: ( $\rho$ ,  $V_m$ ,  $T$ ) Measurements of (Octane + Benzene) at Temperatures from 298.15 K to 328.15 K and at Pressures Up to 40 MPa. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 589 (23 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
47. Nezbeda I.: Aqueous Solutions of Alcohols: What Have We Learnt from Molecular Simulations? 23rd European Symposium on Applied Thermodynamics, Proceedings, pp. 61-62, Cannes, France, 29 May - 01 June 2008.
48. Nezbeda I.: Aqueous Solutions of Alcohols: What Have We Learnt from Molecular Simulations? 7th Liquid Matter Conference, Poster Presentations, p. PB:17, Lund, Sweden, 27 June - 01 July 2008.
49. Nezbeda I.: Aqueous Solutions of Alcohols: What Have We Learnt from Molecular Simulations? ACS Northwest and Rocky Mountain Regional Meeting 2008, Park City, Utah, USA, 15-18 June 2008.
50. Nezbeda I.: Solutions of Alcohols: What Have We Learnt from Molecular Simulations? 18th European Conference on Thermophysical Properties, Pae, France, 31 August - 04 September 2008.
51. Pavlíček J., Wichterle I.: The Correlation of Vapour-Liquid Equilibrium Data: Reliable Evaluation of Temperature Independent Parameters. 23rd European Symposium on Applied Thermodynamics, Proceedings, p. 187, Cannes, France, 29 May - 01 June 2008.
52. Pricl S., Posocco P., Malý M., Lísal M., Fermeglia M.: Beyond Patterns to Mechanisms. Multiscale Molecular Simulations of Nanoparticles/Block Copolymers Self-Assembled Bulk Nanocomposites. AIChE Annual Meeting 2008, Conference Proceedings (4 pp. full text on CD-ROM), p. 404a, Philadelphia, PA, USA, 16-21 November 2008.
53. Předota M., Machesky M.L., Wesolowski D.J., Cummings P.T.: Improved Modeling of the Electric Double Layer at the Rutile (110) Surface using High Temperature Data. 20th International Conference on Chemical Thermodynamics, Book of Abstracts, p. 264, Warsaw, Poland, 03-08 August 2008.
54. Předota M., Vlček L., Wesolowski D.J., Cummings P.T.: Properties of the Solid-Liquid Interface: Beyond the Condensed Layer. 20th International Conference on Chemical Thermodynamics, Book of Abstracts, p. 84, Warsaw, Poland, 03-08 August 2008.
55. Rouha M., Nezbeda I.: The Effect of Cross Interactions on Mixing Properties: non-Lorentz-Berthelot Lennard-Jones Mixtures. 7th Liquid Matter Conference, Poster Presentations, p. PB:25, Lund, Sweden, 27 June - 01 July 2008.
56. Rouha M., Nezbeda I.: Water-Alcohol Mixtures: What Have We Learnt from Molecular Simulation? 7th Liquid Matter Conference, Poster Presentations, p. PB:38, Lund, Sweden, 27 June - 01 July 2008.
57. Sedláková Z., Sauton H., Malijevská I.: Influence of Addition of Ionic Liquid 1-Butyl-3-Methylimidazolium Chloride on Formation of a Solid Compound. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 585 (8 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
58. Sedláková Z., Sauton H., Malijevská I., Hynek V.: Measurements and Prediction Range of Solid Compounds in Systems with Ionic Liquid. 13th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Book of Abstract, Dublin, Ireland, 27-31 July 2008.

59. Škvor J., Nezbeda I.: Percolation Transition in Fluids: Universality of the Wrapping Probability Functions. 7th Liquid Matter Conference, Poster Presentations, p. PI:13, Lund, Sweden, 27 June - 01 July 2008.
60. Wichterle I., Bogdanić G., Erceg-Kuzmić A.: Determination and Evaluation of Phase Equilibrium Data in Polymer + Solvent Systems. 23rd European Symposium on Applied Thermodynamics, Proceedings, pp. 147-148, Cannes, France, 29 May - 01 June 2008.

## Department of Catalysis and Reaction Engineering

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### 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
- Design of new theoretical models for structure-activity relationships
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Temperature programmed techniques in characterization of catalysts
- Preparation of hierarchic nanomaterials

### Applied research

- Catalytic combustion of volatile organic compounds
- Textural characteristics of structural materials

### Research projects

#### Hydrogen oriented underground coal gasification for Europe

(O. Šolcová, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00006)

The project explores the technology for hydrogen production through underground gasification of coal in a dynamic geo-reactor. The process is controlled through purposed dynamic changes in temperature and pressure of the reactants and products. The project addresses CBM usage and CO<sub>2</sub> sequestration in coal deposits. The environmental fingerprint of the technology on air, water and strata stability is evaluated. The locations of demonstration plants are chosen through computer modelling and simulation. Large scale

production of hydrogen from coal is crucial for coal mining industries and will serve the needs of energy, chemistry and transportation sectors of Europe. [Refs. 39-40, 52, 67, 95-97]

### **Hierarchic nanosystems for microelectronics**

(O. Šolcová, joint project with JH IPC, IMC, Institute of Microbiology of the ASCR, v.v.i., Institute of Physics of the ASCR, v.v.i., ICT, CU, UJEP, and Research Institute of Organic Syntheses Pardubice, supported by ASCR, project No. KAN400720701)

Project develops the complex composite systems with precisely defined performance applicable in microelectronics. The individual components will be formed by small arranged particles which will ensure partial function inevitable for functioning of the whole system. These composite structures should be directly applicable as elements of special sensors, photoelectric energy sources, microelectrodes for analytic instruments etc. The general aim of the project is the accumulation of sufficient amount of high-quality experimental data to be applied for design and implementation of practical nanotechnologies. Professionally, the project is focused on the study of preparation of hierarchic nanostructures, inclusive the structural and functional characterization, as well as on prediction of properties by means of mathematical modeling. [Refs. 7-10, 12, 20, 33, 43-45, 50-51, 63-65, 73-76, 90-94, 98]

### **Diffusion coefficients and other transport characteristics of specially shaped porous supports and catalysts**

(O. Šolcová, supported by ASCR, grant No. IAA4072404)

The project develops and verifies a new method for the determination of diffusion coefficients and other transport characteristics of industrial porous solids with non-standard shapes (which guarantee high outer surface to volume ratio). The chromatographic method in SPSC arrangement has been applied. To decrease the number of fitted parameters, the axial dispersion parameter (Peclet number) has been obtained independently of responses of SPSC packed with porous pellets with pores blocked by a suitable liquid - Porofil (nonporous packing). The obtained diffusion coefficients and other transport characteristics have been compared with characteristics from standard textural analyses. [Refs. 21-22, 42, 46, 66, 86-88, 99, 101]

### **Study of factors influencing the activity and selectivity of supported bimetallic transition metal sulfides in HDS and HDN reactions**

(Z. Vít, supported by GA CR, grant No. GA104/06/0870)

Pt/MSA a Pt-Mo/MSA catalysts based on mesoporous silica-alumina (MSA) synthesized by us were studied in simultaneous HDS of thiophene and HDN of pyridine. Monometallic Pt/MSA (up to 2 % Pt) was great at HDS while the promoted Pt-Mo/MSA (0.5 % Pt) showed high HDN. In contrast to alumina, MSA gave more active catalysts due to larger BET area and acidity. Other mesoporous materials such as carriers of Ni phosphide (SBA-15) and Mo, CoMo and NiMo phases (mesoporous alumina) were studied in HDS and HDN of other compounds too, such as benzo- and dibenzothiophene and o-methylaniline. Inhibition of HDS of thiophene by pyridine was studied with Rh-Mo, Ru-Mo and Pd-Mo/alumina and CoMo a NiMo catalysts. Catalysts promoted by noble metals were more resistant to the inhibition than conventional ones and in the presence of pyridine; they were more active in HDS than CoMo. [Refs. 11, 29, 41, 56, 57, 100]

**Synergistic effects in hydrodesulfurization and oxidation reactions**

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

CoMo/Al<sub>2</sub>O<sub>3</sub> catalyst prepared by impregnation of alumina support with cobalt heteropolyoxomolybdate was tested in hydrodesulfurization (HDS) of thiophene, 1-benzothiophene, or light gas oil) under various reaction conditions and reactor arrangements. Its physicochemical properties are also examined. The obtained data are compared with those of two industrial HDS catalysts. [Refs. 23, 89]

**Deposition of oxide catalysts for oxidation of VOC onto preformed support and their modification by nanoparticles of noble metals**

(K. JirátoVá, joint project with ICT, and IIC, supported by GA CR, grant No. GA104/07/1400)

Mode of the promoters (Pt, Pd, La, Ce, K, Li) incorporation into Co<sub>4</sub>MnAl oxidation catalyst and its effect on the activity and selectivity in total oxidation of model VOC (toluene, ethanol) was studied. Addition of potassium showed the highest positive effect on catalyst activity, as it modifies acid-base properties of the catalysts. The effect of LDH precursor crystallinity was studied over the Ni<sub>4</sub>Al<sub>2</sub> system. The highest catalytic activity was found with the system not having too high crystallinity. Formation of LDH precursors on oxidized Al foil under hydrothermal conditions was also studied. [Refs. 13, 28, 31, 35, 36, 58, 78-80]

**Unconventional supports in catalysis over sulfides**

(M. Zdražil, supported by GA CR, grant No. GA104/06/0705)

MoO<sub>3</sub>/TiO<sub>2</sub> catalysts were prepared by conventional impregnation of TiO<sub>2</sub> supports with surface areas of 140, 230, and 407 m<sup>2</sup> g<sup>-1</sup>. The loading of MoO<sub>3</sub> was 2-32 mass%. According to the point of zero charge, the supports were saturated with a molybdena monolayer at approximately 12, 24 and 14 mass%, respectively. Activity in hydrodesulfurization of thiophene increased up to the loading of ~20 mass% and then decreased for all three supports. [Refs. 4, 54]

**Preparation of supported catalysts by slurry impregnation**

(L. Kaluža, supported by GA CR, grant No. GP104/06/P034)

The shaped supports Al<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub> a ZrO(OH)<sub>2</sub> were successfully impregnated by slurry MoO<sub>3</sub>/H<sub>2</sub>O to prepare sharp eggshell concentration profile of Mo, the thickness of which was simply regulated by the nominal amount of MoO<sub>3</sub>. The slurry impregnation thus represented a simple and clear method of the preparation of hydrodesulfurization catalysts, which does not insert NO<sub>3</sub><sup>(-)</sup> and NH<sub>4</sub><sup>(+)</sup> ions into the system, need calcination of catalysts, and distilled water (methanol) evolved during is the only by-product. The highest activities in benzothiophene hydrodesulfurization were obtained after deposition of the promoters (Co, Ni) onto pre-sulfided monolayer Mo catalysts from acetylacetonate precursors. It was found that the monoclinic ZrO<sub>2</sub> (baddeleyite) and tetragonal TiO<sub>2</sub> (anatase) significantly and systematically increase hydrodesulfurization activity of sulfided V, Cr, Mn, Fe, Co, Ni, Mo, Ru, W, and Os species in comparison to conventional Al<sub>2</sub>O<sub>3</sub> support while the activity of sulfided Rh, Pd, Ir, Pt and Re is not influence or is decreased. [Refs. 5-6, 23, 32, 59-62, 89]

**Chemical structures from the analysis of pair density and related quantities**

(R. Ponec, supported by ASCR, grant No. IAA4072403)

The project is a part of longer-term efforts at the systematic exploitation of the pair density as new source of the information about the molecular structure and nature of chemical bond. This density represents the basic theoretical quantity allowing us to describe the behaviour of electron pairs in microscopic systems. In the past several years it was proven to

provide new valuable insights into the role of electron pairing in chemical bond. Especially useful in this respect were found the approaches known as the analysis of domain averaged Fermi holes and the generalized population analysis. These approaches have been applied to the interpretation of the bonding in molecules with complicated bonding pattern like metal-metal bonding, 3-center 4-electron bonding, hypervalence, etc. and to the quantitative characterization of the extended cyclic delocalization in aromatic hydrocarbons. [Refs. 2, 16-19, 25, 27, 38, 85]

### **Advanced catalytic processes and materials**

(J. Hanika, O. Šolcová, joint project with JH IPC, ICT, CU, and UPa, supported by GA CR, grant No. GD203/08/H032)

The concerted project is aimed at a development of new selective catalytic and separation processes for preparation of specialty compounds and materials, which can give rise to a progression in the field of new chemical technologies. The processes in question are stereoselective and regioselective transformations on chiral catalytic centres and processes with significant environmental impact. Coordination of Thesis projects is planned in the field of catalysis, e.g., developed Rh catalysts can be tested in stereospecific polymerizations (CU), asymmetric synthesis (ICT) and hydrocarbonylations; oxidation catalysts can be tested in organic synthesis (ICT, UPa, ICPF), oxidation polymerization (CU) and synthesis of chemical specialties (JH IPC); new mesoporous materials prepared at JH IPC will be used in all other partner laboratories, etc. [Refs. 24, 68-72, 82]

### **International co-operations**

Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification

Delft University of Technology, Delft, Netherlands: Transport characteristics for coal gasification

University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification

Institut Scientifique de Service Public, Liege, Belgium: Transport characteristics for coal gasification

UCG Partnership LTD, Woking, United Kingdom: Transport characteristics for coal gasification

Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification

National Mining University, Dnepropetrovsk, Ukraine: Transport characteristics for coal gasification

Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials

University of Ghent, Ghent, Belgium: Generalized population analysis, theoretical characterization of aromaticity, molecular basis of structure activity relationships

University of Helsinki, Finland: Structure and bonding in metal carbonyls

Chemical Institute of Hungarian Academy of Sciences, Budapest, Hungary: Structure and bonding in metal carbonyls

University of Paris VI, Paris, France: Theory of chemical bond

Institute of Computational Chemistry, University of Girona, Spain: Theory of chemical bond

Institute of Catalysis, Sofia, Bulgaria: Synergistic effects in hydrodesulfurization and oxidation reactions

## Visitors

P. Bultinck, University of Ghent, Belgium  
F. Feixas, University of Girona, Spain  
M. Kohout, Max-Planck Institute Dresden, Germany  
M. Mandado, University of Vigo, Spain

## Teaching

R. Ponec: CU, course "Structure and reactivity"  
P. Schneider, O. Šolcová: ICT, postgraduate course "Texture of porous solids"

## Publications

### Original papers

1. Balcar H., Topka P., Sedláček J., Zedník J., Čejka J.: Polymerization of Aliphatic Alkynes with Heterogeneous Mo Catalysts Supported on Mesoporous Molecular Sieves. *J. Polym. Sci. Part A : Polym. Chem.* 46(7), 2593-2599 (2008).
2. Cooper D.L., Ponec R.: A One-Electron Approximation to Domain Averaged Fermi hole Analysis. *Phys. Chem. Chem. Phys.* 10(9), 1319-1329 (2008).
3. Čapek P., Hejtmánek V., Brabec L., Zikánová A., Kočířík M.: Effective Diffusivities of Gases in a Reconstructed Porous Body. *Chem. Eng. Res. Des.* 86(7), 713-722 (2008).
4. Gulková D., Kaluža L., Vít Z., Horáček J., Macháček E., Zdražil M.: High Surface Area Hydrodesulfurization MoO<sub>3</sub>/TiO<sub>2</sub> Catalysts. *Reac. Kinet. Catal. Lett.*, 94(2), 219-226 (2008).
5. Kaluža L., Gulková D., Šolcová O., Žilková N., Čejka J.: Hydrotreating Catalysts Supported on Organized Mesoporous Alumina: Optimization of Mo Deposition and Promotional Effects of Co and Ni. *Appl. Catal., A* 351(1), 93-101 (2008).
6. Kaluža L., Zdražil M.: The Effect of gamma-Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, and ZrO<sub>2</sub> Supports on Hydrodesulfurization Activity of Transition-Metal Sulfides. *Collect. Czech. Chem. Commun.* 73(8-9), 945-955 (2008).
7. Klusoň P., Drobek M., Kalaji A., Zárubová Š., Krýsa J., Rakušan J.: Singlet Oxygen Photogeneration Efficiencies of a Series of Phthalocyanines in Well-defined Spectral Regions. *J. Photochem. Photobiol., A* 199(2-3), 267-273 (2008).
8. Klusoň P., Drobek M., Krejčíková S., Krýsa J., Kalaji A., Cajthaml T., Rakušan J.: Molecular Structure Effects in Photodegradation of Phenol and Its Chlorinated Derivatives with Phthalocyanines. *Appl. Catal., B* 80(3-4), 321-326 (2008).
9. Klusoň P., Drobek M., Strašák T., Kalaji A.: Photoinduced Catalytic Partial Oxidation of Citronellol with Assistance of PHCs. *React. Kinet. Catal. Lett.* 95(2), 231-238 (2008).
10. Kment Š., Klusoň P., Bartková H., Krýsa J., Churpita O., Čada M., Virostko P., Kohout M., Hubička Z.: Advanced Methods for Titanium (IV) Oxide Thin Functional Coatings. *Surf. Coat. Technol.* 202(11), 2379-2383 (2008).
11. Korányi T.I., Vít Z., Poduval D.G., Ryoo R., Kim H.S., Hensen E.J.M.: SBA-15-Supported Nickel Phosphide Hydrotreating Catalysts. *J. Catal.* 253(1), 119-131 (2008).

12. Matějová L., Schneider P., Šolcová O.: Standard (Master) Isotherms of Alumina, Magnesia, Titania and Controlled-Pore Glass. *Micropor. Mesopor. Mat.* 107(3), 227-232 (2008).
13. Mikulová Z., Jiráťová K., Klempa J., Kovanda F.: Modification of Co-Mn-Al Mixed Oxide with Promoters and Their Effect on Properties and Activity in VOC Total Oxidation. *Collect. Czech. Chem. Commun.* 73(8-9), 1000-1014 (2008).
14. Obalová L., Kovanda F., Jiráťová K., Pacultová K., Lacný Z.: Application of Calcined Layered Double Hydroxides as Catalysts for Abatement of N<sub>2</sub>O Emissions. *Collect. Czech. Chem. Commun.* 73(8-9), 1045-1060 (2008).
15. Pacultová K., Obalová L., Kovanda F., Jiráťová K.: Catalytic Reduction of Nitrous Oxide with Carbon Monoxide over Calcined Co-Mn-Al Hydrotalcite. *Catal. Today* 137(2-4), 385-389 (2008).
16. Ponec R., Cooper D.L., Savin A.: Analytic Models of Domain-Averaged Fermi Holes: A New Tool for the Study of the Nature of Chemical Bonds. *Chem. Eur. J.* 14(11), 3338-3345 (2008).
17. Ponec R., Fias S., Bultinck P., Gutman I., Stankovič S.: O aromaticitě a lokální aromaticitě benzenoidních uhlovodíků. (Hun) On Aromaticity and Local Aromaticity of Benzenoid Hydrocarbons. (Hun) *Magyar Kémiai Folyóirat*, 114(4), 177-182 (2008).
18. Ponec R., Lendvay G., Chavez J.: Structure and Bonding in Binuclear Metal Carbonyls from the Analysis of Domain Averaged Fermi Holes. I Fe<sub>2</sub>(CO)<sub>9</sub> and Co<sub>2</sub>(CO)<sub>8</sub>. *J. Comp. Chem.* 29(9), 1387-1398 (2008).
19. Ponec R., Lendvay G., Sundberg M.: Structure and Bonding in Binuclear Metal Carbonyls from the Analysis of Domain Averaged Fermi holes. Fe<sub>2</sub>(CO)<sub>8</sub>(2-) and Fe<sub>2</sub>(CO)<sub>8</sub>. *J. Phys. Chem. A* 112(40), 9936-9945 (2008).
20. Schneider P., Hudec P., Šolcová O.: Pore-Volume and Surface Area in Microporous-Mesoporous Solids. *Micropor. Mesopor. Mat.* 115(3), 491-496 (2008).
21. Soukup K., Schneider P., Šolcová O.: Comparison of Wicke-Kallenbach and Graham's Diffusion Cells for Obtaining Transport Characteristics of Porous Solids. *Chem. Eng. Sci.* 63(4), 1003-1011 (2008).
22. Soukup K., Schneider P., Šolcová O.: Wicke-Kallenbach and Graham's Diffusion Cells; Limits of Application for Low Surface Area Porous Solids. *Chem. Eng. Sci.* 63(18), 4490-4493 (2008).
23. Spojakina A.A., Jiráťová K., Novák V., Palcheva R., Kaluža L.: Hydrodesulfurization of Different Feeds on CoMo/Al<sub>2</sub>O<sub>3</sub> Catalyst Prepared Using Cobalt Heteropolyoxomolybdate. *Collect. Czech. Chem. Commun.* 73(8-9), 983-999 (2008).
24. Šolcová O., Matějová L., Krejčíková S., Matěj Z., Kužel R., Strýhal Z., Benada O.: Structural Study of Tailored Titania Thin Layers. *Collect. Czech. Chem. Commun.* 73(8-9), 1222-1230 (2008).
25. Cooper D.L., Ponec R.: Anatomy of Bond Formation. Insights from the Analysis of Domain Averaged Fermi Holes in Momentum Space. *Int. J. Quantum Chem.*, submitted.
26. Čapek P., Hejtmánek V., Brabec L., Zikánová A., Kočířik M.: Stochastic Reconstruction of Particulate Media Using Simulated Annealing: Improving Pore Connectivity. *Transp. Porous Media*, in press.
27. Durdevič J., Gutman I., Ponec R.: Verifying the PCP-rule by Five-Center Bond Indices. *J. Serb. Chem. Soc.*, submitted.
28. Galejová K., Obalová L., Jiráťová K., Pacultová K., Kovanda F.: N<sub>2</sub>O Catalytic Decomposition – Effect of Pelleting Pressure on Activity of the Co-Mn-Al Mixed Oxide Catalysts. *Chem. Pap.*, submitted.



29. Gulková D., Yoshimura Y., Vít Z.: Mesoporous Silica-Alumina as Support for Pt and Pt-Mo Sulfide Catalysts; Effect of Pt Loading on Activity and Selectivity in HDS and HDN of Model Compounds. *Appl. Catal., B*, submitted.
30. Hejtmánek V., Čapek P., Brabec L., Zikánová A., Kočířík M.: Určování mikrostrukturních deskriptorů z digitálních snímků pórovitých látek. (Czech) Determination of Microstructural Descriptors from Digital Images of Porous Media. *Chem. Listy*, in press.
31. Jiráťová K., Mikulová J., Klempa J., Grygar T., Bastl Z., Kovanda F.: Modification of Co-Mn-Al Mixed Oxide with Potassium and Its Effect on Deep Oxidation of VOC. *Appl. Catal., A*, submitted.
32. Kaluža L., Zdražil M.: Slurry Impregnation of ZrO<sub>2</sub> Extrudates: Controlled EggShell Distribution of MoO<sub>3</sub>, Hydrodesulfurization Activity, Promotion by Co. *Catal. Lett.*, in press.
33. Kočí K., Obalová L., Matějová L., Plachá D., Jirkovský J., Šolcová O.: Effect of TiO<sub>2</sub> Particle Size on the Photocatalytic Reduction of CO<sub>2</sub>. *Appl. Catal., B*, submitted.
34. Kovanda F., Mašátová P., Novotná P., Jiráťová K.: Formation of Layered Double Hydroxides on Alumina Surface in Aqueous Solutions Containing Divalent Metal Cations. *Clay and Clay Minerals*, submitted.
35. Kovanda F., Rojka T., Bezdička P., Jiráťová K., Obalová L., Pacultová K., Bastl Z., Grygar T.: Effect of Hydrothermal Treatment on Properties of Ni-Al Layered Double Hydroxides and Related Mixed Oxides. *Sol. State Chem.*, in press.
36. Mikulová J., Jiráťová K., Mikulová Z., Klempa J., Kovanda F.: Uranium Promoted Co-Mn-Al-O Catalysts for Oxidation of VOC. *Catal. Today*, submitted.
37. Obalová L., Galejová K., Jiráťová K., Kovanda F.: Effect of Potassium in a Calcined Co-Mn-Al Layered Double Hydroxide on the Catalytic Decomposition of N<sub>2</sub>O. *Appl. Catal., B*, submitted.
38. Ponec R., Fias S., Van Damme S., Bultinck P., Gutman I., Stankovič S.: The Close Relation between Cyclic Delocalization, Energy Effects of Cycles and Aromaticity. *Collect. Czech. Chem. Commun.*, in press.
39. Šolcová O., Matějová L., Hudec P., Schneider P.: Modified BET Equation for Determination of Micropore Pore-volume and Mesopore Surface Area in Microporous-mesoporous Solids. *Stud. Surf. Sci. Catal.*, in press.
40. Topka P., Zub Y.L., Karban J., Šolcová O.: Designing (Al-)SBA-15 Catalyst Pellets with Unique Properties. *Stud. Surf. Sci. Catal.*, in press.
41. Vít Z., Kaluža L., Gulková D., Zdražil M.: Noble Metal Promoted Hydrodesulfurization Catalysts Highly Tolerant to the Inhibition by Pyridine. *J. Catal.*, submitted.

#### Chapters in books

42. Šolcová O., Matějová L., Hudec P., Schneider P.: Possibilities and Limits of Texture Properties Characterization. In: *Sol-Gel Methods for Materials Processing*. (Plinio, I. - Zub, Y.L. - Kessler, V.G., Ed.), pp. 435-440, Springer, Dordrecht 2008.
43. Šolcová O., Matějová L., Klusoň P., Matěj Z., Strýhal Z., Pavlík J., Cajthaml T.: Preparation and Characterization of Thin Nanocrystalline TiO<sub>2</sub> Layers. In: *Sol-Gel Methods for Materials Processing*. (Plinio, I. - Zub, Y.L. - Kessler, V.G., Ed.), pp. 441-446, Springer, Dordrecht 2008.

## Patents

44. Šolcová O., Matějová L., Klusoň P., Cajthaml T.: Způsob přípravy krystalické formy oxidu titaničitého. (Czech) Preparation of TiO<sub>2</sub> Crystalline Phase. Pat. No. PV 2008-400. Applied: 08.06.25.
45. Šolcová O., Matějová L., Matěj Z.: Způsob přípravy oxidu titaničitého. (Czech) Method of Titania Preparation. Pat. No. PV 2008-326. Applied: 08.05.27.
46. Šolcová O., Topka P., Soukup K.: Způsob přípravy a regenerace pelet z křemičitanových a hlinitokřemičitanových mesoporézních molekulových sít a pelety připravené tímto způsobem. (Czech) Method of Pellet Preparation from Siliceous and Aluminosiliceous Mesoporous Molecular Sieves Including Regeneration and Pellets Prepared by this Method. Pat. No. PV 2008-325. Applied: 08.05.27.

## International conferences

47. Bendová M., Klusoň P., Sedláková Z., Wagner Z., Černá I., Vašinová J.: Liquid-Liquid Equilibrium in Quaternary System [bmim][PF<sub>6</sub>] + Water + 1-Methylimidazole + 1-Chlorobutane. 13th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Abstracts, Trinity College Dublin, Ireland, 28-31 July 2008.
48. Čapek P., Hejtmánek V.: Modelling of Multicomponent Mass Transport Phenomena in a Porous Membrane Support using Random Three-Dimensional Pore Networks. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 328-329 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
49. Čapek P., Hejtmánek V.: A Relationship between Pore Shapes and Mercury Porosimetry Curves as Revealed by a Random Pore Network. 8th International Symposium on the Characterisation of Porous Solids, Programme and Abstracts, p. 186, Edinburgh, Great Britain, 10-13 June 2008.
50. Drobek M., Klusoň P., Krýsa J., Kalaji A., Rakušan J.: Effect of Phthalocyanine Molecule Structure on Its Photoinduced Production of Singlet Oxygen Species. 235th ACS National Meeting, Abstracts of Papers, p. ORGN-205, New Orleans, LA, USA, 06-10 April 2008.
51. Floriš T., Klusoň P., Bartek L., Drobek M.: Quarternary Ammonium Salts as Reaction Media for Asymmetric Hydrogenation of Ketoesters. Green Solvents - Progress in Science and Application, Book of Abstracts, p. P 44, Friedrichshafen, Germany, 28 September - 01 October 2008.
52. Floriš T., Klusoň P., Bartek L., Storch J.: Quarternary Ammonium Salts as Reaction Media for Asymmetric Hydrogenation of beta-Ketoesters. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 215-221, Štrbské Pleso, Slovakia, 08-12 September 2008.
53. Galejová K., Obalová L., Jiráťová K., Pacultová K., Kovanda F.: N<sub>2</sub>O Catalytic Decomposition - Effect of Pelleting Pressure on Activity of the Co-Mn-Al Mixed Oxide Catalyst. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 204 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
54. Gulková D., Kaluža L., Vít Z., Horáček J., Macháčková E., Zdražil M.: High Surface Area Hydrodesulfurization MoO<sub>3</sub>/TiO<sub>2</sub> Catalysts. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 1, pp. 97-98 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.

55. Gulková D., Kaluža L., Vít Z., Zdražil M.: Support Effect in Hydrodesulfurization over Ruthenium Sulfide. 40th Symposium on Catalysis, Book of Abstracts, pp. 58-59, Prague, Czech Republic, 03-05 November 2008.
56. Gulková D., Vít Z.: Promotion of Mo/SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> Sulfide Catalyst by Pt; Influence on Activity in Hydrotreating of Model Compounds. 13th Nordic Symposium on Catalysis, Book of Abstracts, pp. 184-185, Göteborg, Sweden, 05-07 October 2008.
57. Gulková D., Vít Z.: Effect of Pt Loading on HDS and HDN Activity of Silica-Alumina Supported Pt-Mo- Sulfide Catalysts. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 244-249, Štrbské Pleso, Slovakia, 08-12 September 2008.
58. JirátoVá K., Mikulová J., Klempa J., Grygar T., Bastl Z., Kovanda F.: Effect of Potassium in Layered Double Hydroxide-related Co-Mn-Al Mixed Oxide Catalyst on Deep Oxidation of VOC. 5th International Conference on Environmental Catalysis, Poster Abstracts, p. 356, Belfast, Great Britain, 31 August - 03 September 2008.
59. Kaluža L., Gulková D., Šolcová O., Žilková N., Čejka J.: Hydrodesulphurization Mo, CoMo and NiMo Catalysts Supported on Organised Mesoporous Alumina. 13th Nordic Symposium on Catalysis, Book of Abstracts, pp. 188-189, Göteborg, Sweden, 05-07 October 2008.
60. Kaluža L., Zdražil M.: The Effect of gamma-Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub> and ZrO<sub>2</sub> Supports on Hydrodesulfurization Activity of Transition-Metal Sulfides. 40th Symposium on Catalysis, Book of Abstracts, pp. 16-17, Prague, Czech Republic, 03-05 November 2008.
61. Kaluža L., Zdražil M.: Slurry Impregnation of TiO<sub>2</sub> and ZrO<sub>2</sub> Extrudates: Controlled Eggshell Distribution of MoO<sub>3</sub>, Hydrodesulfurization Activity, Promotion by Co. 40th Annual Polish Conference on Catalysis, Conference Proceedings, p. 135, Krakow, Poland, 11-15 May 2008.
62. Kaluža L., Zdražil M.: Preparation of Zirconia-Supported Hydrodesulfurisation Catalysts by Slurry Impregnation Method. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 1, pp. 103-104 (9 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
63. Kment Š., Olejníček J., Klusoň P., Čada P., Virostko M., Hubička Z.: Measurement of the Plasma Parameters During the Deposition of Photoactive TiO<sub>x</sub>, TiO<sub>x</sub>:N Thin Films by Means of Low Temperature Multi Hollow Cathode Plasma Jet System Advanced Methods for Titanium (IV) Oxide Thin Film Coatings. 1st International Conference on Thin Films and Porous Materials, Book of Abstracts, p. 56, Zeralda, Algeria, 19-22 May 2008.
64. Kment Š., Olejníček J., Klusoň P., Drobek M., Kužel R., Čada P., Virostko M., Hubička Z.: Preparation of Thin Phthalocyanine Layers and Their Structural and Absorption Properties. 4th International Conference on Technological Advances of Thin Films and Surface Coatings, Book of Abstracts, p. 124, Singapore, Singapore, 13-16 July 2008.
65. Kočí K., Obalová L., Matějová L., Plachá D., Lacný Z.: Size Dependency of Nanocrystalline TiO<sub>2</sub> on Photocatalytic Reactivity Exemplified by CO<sub>2</sub> Photoreduction. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 300-307, Štrbské Pleso, Slovakia, 08-12 September 2008.
66. Kočí K., Obalová L., Matějová L., Šolcová O., Plachá D., Lacný Z.: Size Dependency of Nanocrystalline TiO<sub>2</sub> on Photocatalytic Reactivity Exemplified by CO<sub>2</sub> Photoreduction. 1st Nanomaterials and Nanotechnology Meeting Nano Ostrava 2008, Book of Abstracts, p. 42, Ostrava, Czech Republic, 01-04 September 2008.
67. Kočí K., Obalová L., Matějová L., Šolcová O., Plachá D., Lacný Z.: Size Dependency of Nanocrystalline TiO<sub>2</sub> on Photocatalytic Reactivity Exemplified by CO<sub>2</sub> Photoreduction.

- 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 328 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
68. Krejčíková S., Matějová L., Cajthaml T., Matěj Z., Strýhal Z., Šolcová O.: Preparation and Characterization of Nanoporous Doped Titania Layers for Subsequent Applications. 8th International Symposium on the Characterisation of Porous Solids, Programme and Abstracts, p. 163, Edinburgh, Great Britain, 10-13 June 2008.
  69. Krejčíková S., Matějová L., Cajthaml T., Matěj Z., Strýhal Z., Šolcová O.: Nanoporous Titania Layers for Subsequent Applications. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 704, Praha, Czech Republic, 24-28 August 2008.
  70. Krejčíková S., Matějová L., Matěj Z., Jirkovský J., Šolcová O.: Thin Layers of Titania, Zirconia and Their Mixtures - Preparation and Characterization. 40th Symposium on Catalysis, Book of Abstracts, pp. 47-48, Prague, Czech Republic, 03-05 November 2008.
  71. Krejčíková S., Strýhal Z., Pavlík J., Kužel R., Matějová L., Šolcová O.: Preparation and Characterization of Well-Defined Transition Metal Oxide Thin Films. 1st Nanomaterials and Nanotechnology Meeting Nano Ostrava 2008, Book of Abstracts, p. 84, Ostrava, Czech Republic, 01-04 September 2008.
  72. Krejčíková S., Strýhal Z., Pavlík J., Matějová L., Šolcová O.: Preparation and Characterization of Metal Oxide Thin Films. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 165 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  73. Matějová L., Cajthaml T., Matěj Z., Strýhal Z., Benada O., Šolcová O.: Design of Well-Defined TiO<sub>2</sub> for Photocatalysis. 1st Nanomaterials and Nanotechnology Meeting Nano Ostrava 2008, Book of Abstracts, p. 6, Ostrava, Czech Republic, 01-04 September 2008.
  74. Matějová L., Cajthaml T., Klusoň P., Benada O., Matěj Z., Šolcová O.: Purification of Titania Gels. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 166 (3 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  75. Matějová L., Klusoň P., Cajthaml T., Matěj Z., Šolcová O.: Tailoring of Nanoporous TiO<sub>2</sub> by Calcination or Super-/Sub-critical Fluid Extraction. 8th International Symposium on the Characterization of Porous Solids, Programme and Abstracts, p. 164, Edinburgh, Great Britain, 10-13 June 2008.
  76. Matějová L., Klusoň P., Cajthaml T., Matěj Z., Šolcová O.: Tailoring of Nanoporous TiO<sub>2</sub>. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 418, Praha, Czech Republic, 24-28 August 2008.
  77. Mikulová J., Barbier Jr. J., Rossignol S., Mesnard D., Duprez D., Kappenstein Ch.: Wet Air Oxidation of Acetic Acid over Ruthenium Catalysts Supported on Cerium Based Materials - Influence of Metal and Oxide Crystallite Sizes. 5th International Conference on Environmental Catalysis, Poster Abstracts, p. 353, Belfast, Great Britain, 31 August - 03 September 2008.
  78. Mikulová J., Jirátovej K., Mikulová Z., Klempa J., Kovanda F.: Uranium Promoted Co-Mn-Al-O Catalysts for Oxidation of VOC. IX. Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 338-343, 6, Štrbské Pleso, Slovakia, 08-12 September 2008.
  79. Mikulová Z., Jirátovej K., Klempa J., Kovanda F.: Modification of Co-Mn-Al Mixed Oxide with Promoters and Their Effect on Properties and Activity in VOC Total Oxidation. 40th Symposium on Catalysis, Book of Abstracts, pp. 52-53, Prague, Czech Republic, 03-05 November 2008.
  80. Mikulová Z., Jirátovej K., Kovanda F., Klempa J.: Modified Co<sub>4</sub>MnAl Oxidic Catalysts: Effect of Modification on Properties and Catalytic Activity in VOC Oxidation. 35th

- International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 158 (6 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
81. Mikulová J., Rossignol S., Barbier Jr. J.: Wet Air Oxidation of Acetic Acid Catalyzed by Platinum Supported over Cerium (Mixed) Oxide. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 257 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  82. Morozová M., Klusoň P., Šolcová O., Krýsa J., Zlámal M., Steck T.: Preparation and Photoelectrochemical Evaluation of Titania Based Thin Layers. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 333-336, Štrbské Pleso, Slovakia, 08-12 September 2008.
  83. Obalová L., Jirátovej K., Galejová K., Kovanda F.: Effect of Potassium in Calcined Co-Mn-Al Layered Double Hydroxide on Catalytic Decomposition of N<sub>2</sub>O. 5th International Conference on Environmental Catalysis, Book of Abstracts, p. 177, Belfast, Great Britain, 31 August - 03 September 2008.
  84. Obalová L., Kovanda F., Jirátovej K., Pacultová K., Lacný Z.: Application of Calcined Layered Double Hydroxides as Catalysts for Abatement of N<sub>2</sub>O Emissions. 40th Symposium on Catalysis, Book of Abstracts, pp. 54-55, Prague, Czech Republic, 03-05 November 2008.
  85. Ponec R., Chaves J.: Structure and Bonding in Binuclear Metal Carbonyls from the Analysis of Domain Averaged Fermi hole. VIII Girona Seminar on Aromaticity: Basics and Applications, Book of Abstracts, p. 30, Girona, Spain, 07-10 July 2008.
  86. Soukup K., Rogut J., Ludwik-Pardala M., Wiatkowski M., Šolcová O.: Metal Materials for Hydrogen Storage. 40th Symposium on Catalysis, Book of Abstracts, pp. 73-74, Prague, Czech Republic, 03-05 November 2008.
  87. Soukup K., Schneider P., Šolcová O.: Measurements of Intraparticle Diffusion by Liquid Chromatography. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 706, Praha, Czech Republic, 24-28 August 2008.
  88. Soukup K., Schneider P., Šolcová O.: Liquid Chromatography for Determination of Effective Diffusion Coefficients. 8th International Symposium on the Characterization of Porous Solids, Programme and Abstracts, p. 192, Edinburg, Great Britain, 10-13 June 2008.
  89. Spojakina A.A., Jirátovej K., Novák V., Palcheva R., Kaluža L.: Hydrodesulfurization of Different Feeds on CoMo/Al<sub>2</sub>O<sub>3</sub> Catalyst Prepared Using Cobalt Heteropolyoxomolybdate. 40th Symposium on Catalysis, Book of Abstracts, pp. 41-42, Po06, Prague, Czech Republic, 03-05 November 2008.
  90. Šolcová O., Hudec P., Součková H., Šnajdaufová H., Matějová L.: The Modified BET Equation for Correct Determination of Texture Properties in Microporous-Mesoporous Materials. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 164 (6 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  91. Šolcová O., Matějová L., Hudec P., Schneider P.: Modified BET Equation for Determination of Micropore Pore Volume and Mesopore Surface Area in Microporous-Mesoporous Solids. 8th International Symposium on the Characterization of Porous Solids, Programme and Abstracts, p. 103, Edinburg, Great Britain, 10-13 June 2008.
  92. Šolcová O., Matějová L., Hudec P., Schneider P.: The Correct Determination of Micropore Pore Volume and Mesopore Surface Area in Microporous-Mesoporous Solids. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 705, Praha, Czech Republic, 24-28 August 2008.
  93. Šolcová O., Matějová L., Hudec P., Schneider P.: The Correct Determination of Texture Properties in Microporous-Mesoporous Solids. 1st Nanomaterials and Nanotechnology

- Meeting Nano Ostrava 2008, Book of Abstracts, p. 7, Ostrava, Czech Republic, 01-04 September 2008.
94. Šolcová O., Matějová L., Krejčíková S., Matěj Z., Kužel R., Strýhal Z.: Structural Study of Tailored Titania Thin Layers. 40th Symposium on Catalysis, Book of Abstracts, pp. 25-26, 25, Praha, Czech Republic, 03-05 November 2008.
  95. Topka P., Balcar H.: MoO<sub>3</sub> Supported on Mesoporous Silica - New Highly Active Catalyst for Olefin Metathesis. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, pp. 430-431 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
  96. Topka P., Klusoň P., Krejčíková E., Šolcová O.: Designing of (Al)-SBA-15 Catalyst Pellets with Unique Properties. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 167 (3 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  97. Topka P., Klusoň P., Soukup K., Schneider P.: (Al)-SBA-15 with Unique Properties for Friedel-Crafts Alkylation. 8th International Symposium on the Characterization of Porous Solids, Programme and Abstracts, p. 154, Edinburgh, Great Britain, 10-13 June 2008.
  98. Topka P., Klusoň P., Šolcová O.: Self-supporting Pellets from (Al)-SBA-15 Molecular Sieve. 1st Nanomaterials and Nanotechnology Meeting Nano Ostrava 2008, Book of Abstracts, p. 9, Ostrava, Czech Republic, 01-04 September 2008.
  99. Topka P., Zub Yu.L., Šolcová O.: Self-supporting Pellets from (Al)-SBA-15. 40th Symposium on Catalysis, Book of Abstracts, pp. 75-76, Prague, Czech Republic, 03-05 November 2008.
  100. Vít Z.V., Gulková D.G.: Effect of Pt Loading on HDS/HDN Activity of Pt Catalysts Supported on Mesoporous Silica-Alumina. 13th Nordic Symposium on Catalysis, Book of Abstracts, pp. 202-203, Göteborg, Sweden, 05-07 October 2008.
  101. Zub Yu.L., Šolcová O.: Use of Physical Methods for Establishment of the Surface Layer Structure in Functionalized Mesoporous Silicas. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, pp. 421-422 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.

## Department of Multiphase Reactors

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### Fields of research

- Multiphase fluid dynamics and transport phenomena in different types of gas-liquid, liquid-solid or gas-liquid-solid systems
- Sedimentation of ensembles of polydisperse particles, deposit structure
- Flow of microdispersions and liquids with complex rheological behaviour
- Electrodiffusion diagnostics of the flow

### Research projects

#### Continuous fermentation of alcohol-free beer

(M. Růžička, joint project with ICT, supported by GA CR, grant No. GA104/06/1418)

The goal of this project is the investigation of the rheological properties and hydrodynamic behaviour of a bed of carrier particles for supporting biomass in a gas-liquid-solid three-phase system. The particles are the spent grains, because of availability and low price. They form a bed ('sludge blanket') in the fermentor that tend to sediment and settle at the bottom. The fermentor is flown through the liquid phase with a recycle, to keep the bed in a quasi-fluidized state, which is required for the fermentation purpose. Occasionally, it is also sparger with gas, for technological reasons. Our goal is to find the values of control parameters when the bed neither settle nor escape from the reactor. [Refs. 5, 8, 14, 31, 34, 39-42, 45, 47]

#### Analysis of hydrodynamic forces acting on bubbles by PIV measurements

(J. Vejražka, supported by ASCR, grant No. IAA200720801)

The liquid flow in proximity of bubbles is studied experimentally by using the time-resolved particle image velocimetry and high-speed flow visualizations. The measured velocity field will be treated in order to get information on the forces acting on bubbles in different flow situations. The calculation and analysis of the viscous dissipation and inertia of liquid in motion will be performed for various situations both in pure liquids and in surfactant solutions. The results will enlarge the knowledge of bubble flow dynamics, required to improve computational models used for the prediction of macroscopic two-phase flows.

[Refs. 20-21, 45, 47, 48]

**Hydrodynamics of bubble-particle interactions under liquid circulation**

(M. Zedníková, supported by ASCR, grant No. KJB200720801)

The project deals with bubble-particle interactions under liquid circulation. Theoretical description exists only for small particle-large bubble interactions, used in mineral flotation. If the objects proportion is inverted, the mechanism of interaction is no longer fully understood. Thus, the objectives of the project are to study: i) small bubble-large particle interactions under liquid circulation and ii) interaction of more bubbles with a particle and formation of stable bubbles-particle aggregate. The bubble trajectory, velocity, momentum and deformation during impact are obtained by high speed camera visualization and the liquid velocity flow field is measured by PIV. The experimental data will create a base for theoretical description of bubble-particle interactions. [Refs. 9, 20-22]

**Effect of bubble size on stability of homogeneous bubbly layer**

(M. Večeř, supported by GA CR, grant No. GP104/06/P287)

The goal of the project is to investigate experimentally the effect of the size of bubbles on the stability of the homogeneous flow regime in bubble column reactors, and its transition to the heterogeneous flow regime. The former regime lack large-scale motions of the two-phase mixture in the column, while convective currents ('circulations') set in, when loses the stability. There is a theoretical concept developed of the regime transition that is to be verified by measurements. This forms the core of this project. [Refs. 5, 29-31, 33, 35, 36, 44-48, 50-52]

**Transport and reaction processes in complex multiphase systems**

(J. Drahoš, joint project with ICT and UPa, supported by GACR, grant No. GD104/08/H055)

Project is focused on training of doctoral students in the field of chemical engineering via targeted research in modern branches of chemical, pharmaceutical, biological and process industries with emphasis on research in new areas such as micro- and nanotechnologies and material engineering. It includes theoretical and experimental work of 20 students of Chemical Engineering Departments at ICT and UPa, and at ICPF. Particular research programmes involve 16 areas from microsystems to industry-scale processes. Project will be led by 18 supervisors. The training includes both general courses on mathematical modeling, statistical analysis and methodology of scientific work, and courses specialized on specific research fields. Students will take part in national and international projects of cooperation with major research laboratories. The project output will be publications in impacted international journals, presentations at conferences and special workshops with lectures by students, supervisors and invited specialists, published in proceedings. [Refs. 9, 28-31, 37, 38, 41]

**Integrated multiscale process units with locally structured elements (IMPULSE)**

(J. Hanika, V. Jiříčný, J. Drahoš, 6th FP integrated project, Priority 3 NMP, supported by EU under Contract No. 011816-2)

The objective of IMPULSE project is effective, targeted integration of innovative process equipment such as microreactors, heat exchangers, thin-film devices and other micro components to attain radical performance enhancement for whole process systems in chemical production. We are involved in the application of electrodiffusion sensors for the experimental flow diagnostics in microreactors. Another our activity consists in the implementation of numerical simulations for the prediction of two-phase flows in narrow channels. We also participate in the workpackage dealing with the results dissemination.



**CFD-RANS supported prognoses to growth conditions in bioreactors**

(M. Fialová, bilateral co-operation with Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria)

The CFD model of bubble column was verified by experimental data. Bubble column flow field calculated numerically was used in selection of bubble-bed structural models. Results obtained by CFD modeling were employed to analyze oxygen availability for aerobic cell growth in a bio-fluid in bubble column bioreactors. [Refs.12, 19]

**Presidency of the European Federation of Chemical Engineering (EFCE)**

(J. Drahoš, supported by MEYS, INGO project No. LA 319)

The EFCE is one of the most important institutions in the field of chemistry. Prof. Jiří Drahoš successfully served for two years as its President. In September 2007 he has been re-elected as the President for the period 2008-2009. Together with Prof. Růžička, he also participated at the activities of the EFCE Working Party Multiphase Fluid Flow.

**Development of micro-bubble fluid chamber for tissue engineering bioreactor**

(M. Růžička, joint project with Kyushu University Japan, supported by MEYS, KONTAKT project No. ME 952)

Objective of this project is to design a novel bioreactor for tissue engineering. The conventional tissue engineering uses so-called scaffolds as a supporting structure, into which the cells are seeded. The novel bioreactor will have scaffold-less design based on a flow chamber equipped with a device for producing micro bubbles. The tissue growth will be controlled by means of accurately setting the flow conditions in this chamber, i.e. flow of the culture medium and content of micro bubbles in it. [Refs. 41-43, 48, 49, 62]

**Research into small-scale structure of gas-liquid systems with optical probe**

(M. Růžička, joint project with LEGI Grenoble, supported by ASCR and CNRS France, Project No. 11-20213)

This project gives us the possibility to use French probe technique for detailed study of fine structure of multiphase mixtures, on our own gas-liquid systems. Simultaneous measurements of bubble concentration, bubble velocity and bubble size are available because of original construction of monofiber probe. The probe does not much affect the flow structure due to its small proportion (fiber diameter like 150 microns). Study of local properties in multiphase systems allows us to understand its structure on small scales. This knowledge will lead to calibration of macroscopic theories necessary for description of real systems. [Refs. 45, 47]

**Hydrodynamics and transport phenomena in multiphase systems: from microscale to macroscale**

(M. Růžička, joint project with TU Ostrava, supported by GA CR, grant No. GA104/07/1110)

The essence of the research project is the investigation into the basic physical mechanisms involved in hydrodynamics and transport phenomena in complex multiphase systems. Transport of mass and momentum in both two-phase systems (gas-liquid) and three-phase systems (gas-liquid-solid) will be studied. The stress is put on the momentum transfer between the phases, i.e. on the hydrodynamics of multiphase flows. Hand in hand with the understanding the multiphase motion, the mass transfer phenomena will be explored. The typical feature of the multiphase systems is the existence of a microstructure, given by the presence and configuration of the dispersed particles. The microstructure has a multi-scale nature and determines the system rheology. The project is aimed at resolving the relation

between the microstructure and the macroscopic behaviour of the multiphase systems. [Refs. 3, 5, 8-10, 14, 18, 20-22, 28-31, 34, 37-42, 45, 47, 50]

### **Hydrodynamic concept of stromatactis formation in geology**

(M. Růžička, joint project with Institute of Geology of the ASCR, v.v.i., supported by ASCR, grant No. IAAX 00130702)

The stromatactis cavities are present in fine-grained carbonate sediments in the nature, forming the specific shapes and reticulate arrays. However, the mechanisms behind the origin of these cavities are subjects of heated discussions in geology for 125 years. Numerous biotic and abiotic factors were considered, but with unclear results. Most recently, our team produced a critical analysis of these sedimentary structures and formulated a new hypothesis that these cavities would likely originate during the rapid deposition of extremely polydisperse and multimodal granular mixtures. Although the first experiments simulated the production of these cavities with a considerably high level of similarity, there is a lot of work to be done if we wish really explain these unique phenomena in terms of hydrodynamics. The proposed interdisciplinary study is novel, and the results would be fundamental for sedimentology and hydrodynamics, with possible implications in related technologies. [Refs. 8, 14, 28, 30, 31]

### **Effect of the surface roughness, ohmic resistance, and electrode kinetics on autocalibration of electrodiffusion friction probes**

(O. Wein, supported by GACR, grant No. GA104/08/0428)

Experimental part of the project consists in studying fast transient processes driven by a step change of voltage in electrolytic microcells. In the first year of the project, an experimental set-up (electrolytic cells, working electrodes, measuring and controlling hardware) were prepared and tested. The programs for PC-driven process control and data acquisition, written under LabView, were prepared and tested. This preparatory activity is documented in a series of 3 research reports. The related results in electrodiffusion diagnostics of flow were published. [Refs. 13, 43, 49]

## **International co-operations**

CRTT, Saint Nazaire, France: Backward-facing step flows, Microfluidics  
LEGI / IMG, Grenoble, France: Bubble columns, Optical probes  
Institute of Fluid Mechanics, Toulouse, France: Hydrodynamic interactions of bubbles  
Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow  
University of Thessaly, Volos, Greece: Liquid film flows  
Aristotle University, Thessaloniki, Greece: Rheology of nanofluids  
University of Minho, Braga, Portugal: Multiphase bubble bed reactors  
University of Porto, Portugal: Hydrodynamics of g-l-s systems  
Slovak Technical University, Bratislava, Slovakia: Mass transfer in bubble columns  
Institute of Chemical Engineering, BAS, Sofia, Bulgaria: Gas-liquid reactors  
Institute of Thermophysics, RAS, Russia: Diagnostics of multiphase flows  
Twente University, Twente, The Netherlands: Hydrodynamics of bubbly flow  
Worcester Polytechnic Institute, Worcester, USA: CFD  
Technology Institute, SINTEF, Trondheim, Norway: Bubble columns  
Kyoto University, Japan: Hydrodynamics of bubbly flow

Kobe University, Japan: Hydrodynamics of bubbly flow  
Kyushu University, Fukuoka, Japan: Hydrodynamics of bubbly flow  
ITT Flygt AB, Sundbyberg, Sweden: CFD

## Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)  
P. Stanovský: Kyushu University, Fukuoka, Japan (1 month)  
P. Stanovský: Shizuoka University, Hamamatsu, Japan (1 month)

## Visitors

A. Sato, Kyushu University, Japan  
T. Sanada, Kyushu University, Fukuoka, Japan  
P. Sechet, University of Grenoble, France  
S. Paras, Aristotle University of Thessaloniki, Greece  
A. Mouza, Aristotle University of Thessaloniki, Greece  
N. Kazakis, Aristotle University of Thessaloniki, Greece  
N. Ait Mouheb, CRTT, Saint-Nazaire, France  
S.D. Vlaev, BAS, Sofia, Bulgaria  
J. Comiti, University of Nantes, France

## Teaching

J. Drahoš: ICT, postgraduate course "Multiphase reactors"  
M. Růžička: ICT, postgraduate courses "Multiphase reactors", "Multiphase hydrodynamics"  
J. Tihon: ICT, postgraduate course "Drops, bubbles, and particles"  
M. Večeř: TU Ostrava, courses "Process engineering" and "Chemical process modeling"  
J. Havlica: UJEP, courses "Introduction to MATLAB" and "Mathematics"

## Publications

### Original papers

1. Huchet F., Havlica J., Legentilhomme P., Montillet A., Comiti J., Tihon J.: Use of Electrochemical Microsensors for Hydrodynamics Study in Crossing Microchannels. *Microfluid. Nanofluid.* 5(1), 55-64 (2008).
2. Kristiawan M., Sobolík V., Al-Haddad M., Allaf K.: Effect of Pressure-Drop Rate on the Isolation of Cananga Oil Using Instantaneous Controlled Pressure-Drop Process. *Chem. Eng. Process.* 47(1), 66-75 (2008).

3. Paglianti A., Fugasová M., Montante G.: A Simple Model for Power Consumption in Gassed and Boiling Stirred Vessels. *AICHE J.* 54(3), 646-656 (2008).
4. Rochová K., Sovová H., Sobolík V., Allaf K.: Impact of Seed Structure Modification on the Rate of Supercritical CO<sub>2</sub> Extraction. *J. Supercrit. Fluids* 44(2), 211-218 (2008).
5. Růžička M., Večeř M., Orvalho S.P., Drahoš J.: Effect of Surfactant on Homogeneous Regime Stability in Bubble Column. *Chem. Eng. Sci.* 63(4), 951-967 (2008).
6. Sobolík V., Wein O.: The Levich Problem with an Eccentric Segmented Electrode on Rotating Disk. *Russ. J. Electrochem.* 44(4), 424-433 (2008).
7. Sobolík V., Wein O.: Zadacha Levicha: Ekstsentricheskiei Segmentnyi Elektrod na Vrashchayushchemsya Diske. (Russ). *Elektrokhimiya* 44(4), 459-469 (2008).
8. Šimčík M., Růžička M., Drahoš J.: Computing the Added Mass of Dispersed Particles. *Chem. Eng. Sci.* 63(18), 4580-4595 (2008).
9. Vejražka J., Fugasová M., Stanovský P., Růžička M., Drahoš J.: Bubbling Controlled by Needle Movement. *Fluid Dyn. Res.* 40(7-8), 521-533 (2008).
10. Moucha T., Linek V., Erokhin K., Rejl J.F., Fugasová M.: Improved Power and Mass Transfer Correlations for Design and Scale-up of Multi-Impeller Gas-Liquid Contactors. *Chem. Eng. Sci.*, in press.
11. Růžička M., Bunganič R., Drahoš J.: Meniscus Dynamics in Bubble Formation. *Chem. Eng. Res. Des.*, in press.
12. Staykov P., Fialová M., Vlaev S.D.: Bubble-Bed Structural Models for Hybrid Flow Simulation: An Outlook Based on a CFD-Generated Flow Image. *Chem. Eng. Res. Des.*, in press.
13. Tihon J., Pěnkavová V., Pantzali M.: The Effect of Inlet Pulsations on the Backward-Facing Step Flow. *Int. J. Heat Fluid Flow*, submitted.

#### Review papers

14. Růžička M.: On Dimensionless Numbers. *Chem. Eng. Res. Des.* 86(8), 835-868 (2008).

#### Patents

15. Hájek M., Drahoš J.: Method of Drying of Book and Similar Paper Material and Equipment for Its Processing. Pat. No. EP 1441191. Applied: 22.12.2003, Granted: 08.02.13.

#### International conferences

16. Cvetinovič D., Tihon J., Vejražka J., Drahoš J.: Numerical Modelling of Turbulent Circular Air Free Jet and Its Experimental Validation. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, pp. 899-900 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
17. Cvetinovič D., Tihon J., Vejražka J., Drahoš J.: Unsteady Numerical Modelling of Turbulent Circular Air Jet Impinging on a Flat Surface and Its Experimental Validation. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, pp. 901-902 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
18. Fialová M., Orvalho S.P., Fugasová M., Růžička M., Drahoš J.: The Use of the Ideal and Non-ideal Dynamic Pressure Step Method for  $k_{La}$  Measurement and Effect of Electrolyte Addition on Gas Holdup and  $k_{La}$  in Bubble Column. 18th International Congress of

- Chemical and Process Engineering CHISA 2008, Summaries 3, p. 858, Praha, Czech Republic, 24-28 August 2008.
19. Fialová M., Staykov P., Vlaev S.D.: Interpretation of CFD-Generated Bubble Swarms Oscillation for Bubble Column Bioreactor Performance Analysis. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 859 (11 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
  20. Fugasová M., Vejražka J., Růžička M., Drahoš J.: Hydrodynamics of Bubble Bouncing on a Wall, Experiment and Modelling. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 878 (9 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
  21. Fugasová M., Vejražka J., Růžička M., Drahoš J.: On a Bubble Bouncing on a Wall in Various Liquid Phases. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 304, Tatranské Matliare, Slovakia, 26-30 May 2008.
  22. Fugasová M., Vejražka J., Růžička M., Drahoš J.: Hydrodynamics of Bubble Bouncing on a Wall, Experiment and Modelling. XXII. Symposium on Anemometry, Proceedings, pp. 20-27, Holany-Litice, Czech Republic, 03-04 June 2008.
  23. Gogová Z., Hanika J.: Design of Gas-Lift Reactor for Catalytic Oxidation. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 1, p. 248, Praha, Czech Republic, 24-28 August 2008.
  24. Gogová Z., Hanika J.: Model Aided Design of Gas-Lift Reactor for Oxidation Reaction with Fast Reversible Catalyst Deactivation. 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, Book of Abstracts, p. 711 (6 pp. full text on CD-ROM), Braga, Portugal, 04-06 September 2008.
  25. Gogová Z., Hanika J.: Purpose Tailored Design of Gas-Lift Reactor. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 271 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  26. Hladil J., Koptíková N., Lisá L., Čejchan P., Růžička M., Kulaviak T., Adamovič J., Janečka J., Večeř M., Drahoš J., Havlica J.: Stromatactis and Stromatactum Pattern Formation in Sediment: Constraints from Fluid Mechanics and Rheology and Implications for Environments, Sedimentary Architecture and Cyclostratigraphy. International Conference Global Alignments of Lower Devonian Carbonate and Clastic Sequences, Book of Abstracts, pp. 36-40, Tashkent, Uzbekistan, 25 August - 03 September 2008.
  27. Kříšťál J., Havlica J., Jiříčný V.: Hydrodynamic Characterization of Electrochemical Microreactor. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 5, p. 1726 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
  28. Kulaviak L., Růžička M., Drahoš J., Hladil J.: Cavities Formation in Sedimentary Deposits. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 241, Tatranské Matliare, Slovakia, 26-30 May 2008.
  29. Kulaviak L., Večeř M., Růžička M., Drahoš J., Hladil J.: Viscosity Characteristic of Model Suspensions. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 312, Tatranské Matliare, Slovakia, 26-30 May 2008.
  30. Kulaviak L., Večeř M., Růžička M., Drahoš J., Hladil J.: Viscosity Characteristics of Geological Suspensions. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 927, Praha, Czech Republic, 24-28 August 2008.
  31. Kulaviak L., Večeř M., Růžička M., Drahoš J., Hladil J.: Flow Behavior of Model Suspensions. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 823, Praha, Czech Republic, 24-28 August 2008.

32. Mouheb N.A., Sollicec C, Montillet A., Comiti J., Legentilhomme P., Havlica J.: Numerical Study of the Flow and Mass Transfer in Micromixers. 6th International ASME Conference on Nanochannels, Microchannels and Minichannels ICNMM2008, Proceedings, p.1(6 pp. full text on CD-ROM), Darmstadt, Germany, 23-25 June 2008.
33. Obalová L., Večeř M.: Thermal Dehydration of Phthalic Acid. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 97, Tatranské Matliare, Slovakia, 26-30 May 2008.
34. Orvalho S.P., Martín M., Fijasová M., Růžička M., Drahoš J.: Aspects of Coalescence of Pairs of Bubbles. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 879, Praha, Czech Republic, 24-28 August 2008.
35. Smutná K., Wichterle K., Večeř M.: Study on Behavior of Bubbles Rising in Various Liquids. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 875 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
36. Smutná K., Wichterle K., Večeř M.: Oscillation Frequency of Bubbles Moving Periodically in Various Liquids. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 196 (6 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
37. Stanovský P., Fijasová M., Růžička M., Drahoš J., Sanada T., Shiota M., Sato A., Watanabe A.: Experimental Investigation of in Line Rising Bubbles. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 876, Praha, Czech Republic, 24-28 August 2008.
38. Stanovský P., Růžička M., Drahoš J., Sanada T., Shiota M., Sato A., Watanabe M.: Interactions between Bubbles Rising in Line. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 234, Tatranské Matliare, Slovakia, 26-30 May 2008.
39. Šimčík M., Havlica J., Růžička M., Drahoš J.: CFD Simulation of Laboratory Scale Airlift Reactor Hydrodynamics: Case Study. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 310, Tatranské Matliare, Slovakia, 26-30 May 2008.
40. Šimčík M., Havlica J., Růžička M., Drahoš J., Teixeira J., Brányik T., Novák P., Baszczyński M., Kuřec M.: Euler-Euler Simulation of Gas-liquid and Gas-liquid-solid Airlift Reactors: Case Study. 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, Book of Abstracts, pp. 264-265, Braga, Portugal, 04-06 September 2008.
41. Šimčík M., Kulaviak L., Havlica J., Růžička M., Drahoš J., Teixeira J.: Gas Holdup in Laboratory Scale Bubble Column: CFD Simulations vs. Measurements. 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, Book of Abstracts, pp. 453-454, Braga, Portugal, 04-06 September 2008.
42. Šimčík M., Růžička M., Havlica J., Drahoš J., Teixeira J.: CFD Simulation of Hydrodynamics of Rectangular External Loop Airlift Reactor. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 862, Praha, Czech Republic, 24-28 August 2008.
43. Tihon J., Pěnkavová V.: Experimental Investigation of the Near-Wall Flow behind a Backward-Facing Step. 7th EUROMECH Fluid Mechanics Conference, Abstracts, p. 336, Manchester, Great Britain, 14-18 September 2008.
44. Tihon J., Večeř M., Pěnkavová V.: Rheology of Nanofluids. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 301, Tatranské Matliare, Slovakia, 26-30 May 2008.

45. Večeř M., Kabieszová J., Sechet Ph., Vejražka J., Orvalho S.P., Cartellier A., Růžička M.: Interaction of Bubble with Optical Probe Sensor. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 198, Tatranské Matliare, Slovakia, 26-30 May 2008.
46. Večeř M., Tihon J., Pěnkavová V.: Rheology of Aqueous Nanosuspensions. 1st Nanomaterials and Nanotechnology Meeting Nano Ostrava 2008, Book of Abstracts, p. PP-37, Ostrava, Czech Republic, 01-04 September 2008.
47. Večeř M., Vejražka J., Sechet P., Orvalho S.P., Růžička M., Cartellier A., Drahoš J.: Validation of Optical Probes - Fiction and Reality. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, pp. 798-799 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
48. Vejražka J., Večeř M., Orvalho S.P., Sechet P., Cartellier A.: Optical Probes and Their Measurement Precision. (Czech). XXII. Symposium on Anemometry, Proceedings, pp. 109-118, Holany, Czech Republic, 03-04 June 2008.
49. Wein O.: Directional Characteristics of Multisegment ED Probes under Apparent Wall-Slip (AWS) Effect. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 921, Praha, Czech Republic, 24-28 August 2008.
50. Wichterle K., Raška P., Večeř M.: Bubbles Rising in Non-uniform Velocity Field. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 311 (4 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
51. Wichterle K., Raška P., Večeř M., Růžička M.: Self-organization of a Group of Large Rising Bubbles. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 795 (5 pp. full text on CD-ROM), p. 795, Praha, Czech Republic, 24-28 August 2008.
52. Wichterle K., Smutná K., Večeř M.: Oscillation of the Shape of Rising Bubbles. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 874 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.

## Department of New Processes in Chemistry and Biotechnology

Head: J. Čermák  
Deputy: G. Kuncová  
Research staff: L. Červenková Šťastná, Y. Maléterová, M. Pošta, S. Šabata, J. Včelák  
Part time: M. Czakóová, J. Hetflejš, F. Kaštánek  
Technical staff: J. Kubešová, R. Lehnert, J. Zavázalová  
PhD students: J. Bolyó, A. Krupková, R. Rychtáriková, J. Storch, T. Strašák

### Fields of research

- Bioremediation of organic pollutants in soil and sewage
- Immobilization of biocatalysts, living cells or enzymes, into organic or organic-inorganic matrices by sol-gel process
- Application of immobilized biocatalysts in optical sensors
- Polymeric antidegradants immobilized on poly(siloxanes)
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphasic media
- Carbosilane dendrimers

### Applied research

- Complex dehalogenation of PCB contaminated soils, waste water and oils

### Research projects

**The research and verification of the method of catalytic dehalogenation of underground water from industrial sources by bimetallic permeable barriers**  
(F. Kaštánek, supported by MIT, IMPULS project No. FI-IM3/050)

The response rate of the reductive dehalogenation of halogenated (aliphatic chlorinated hydrocarbons) and polyhalogenated organic compounds (PCB) was studied. Experiments were realized in water emulsions with bimetallic catalysts (common metal and palladium, concentration of palladium was 0.05 – 0.2 %). Palladium was present in the form of isolated isles on the elementary common metal surface: Pd/Fe, Pd/Al, Pd/Mg, Pd/Ni and Pd/Zn. The method of the catalyst preparation was optimized. The best efficiency was achieved with the three-phase catalyst type Pd-Fe-C. In the gray iron carbon was present in the graphite form as inclusions in the concentration to 4 %. Reductive effects of this catalyst are based on the transfer of electrons which are generated by the corrosion of the common metal and by the function of the system as an electrolytic cell. This catalyst is economically and ecologically



advantageous since his durability reached six months. The efficiency was tested in the real decontamination process of water contaminated by polychlorinated ethanes and ethylenes. [Refs. 7, 8]

### **The structure and synthetic applications of transition metal complexes**

(J. Čermák, joint project with JH IPC, CU, and ICT, supported by MYES, project No. LC06070)

Modular iterative synthesis of helicenes up to hexahelicene was developed, the key feature being transition metal catalyzed cycloisomerization of alkynyl substituted biphenylnaphthalenes. Two types of rhodium diphosphinoazine complexes were synthesized and thoroughly characterized, rhodium(I) square planar carbonyl complexes and rhodium(III) octahedral halo complexes. Dynamic features in these compounds were studied by NMR spectroscopy. Palladium(II) aryl-amido diphosphinoazine complexes with an unsymmetrical ligand coordination mode were prepared and characterized including x-ray diffraction. Peripheral substitution of carbosilane dendrimers by cyclopentadienes and cyclopentadienyl complexes was studied. Novel alkene and diene complexes with  $[(C_5Me_4C_nF_{2n+1})Rh]$  fragment were synthesized for potential applications in catalytic reactions, and their structure was determined including an x-ray structure of a dicarbonyl rhodium(I) complex. [Refs. 3, 5, 10, 13, 14, 20]

### **Singlet oxygen producing sensitizers on solid inorganic hosts: photodisinfecting materials and probes**

(G. Kuncová, joint project with IIC, JH IPC, and CU, supported by GA CR, grant No. GA203/06/1244)

Sol-gel derived mesoporous antimicrobial biomaterials were prepared by entrapment of hydrophilic and hydrophobic porphyrines into polysilsesquioxanes. Mesoporous structure of novel polysilsesquioxane matrices increased their antimicrobial activity as compared to microporous silica gel prepared from tetramethoxysilane. Novel method of biotoxicity evaluation of singlet oxygen generated by immobilized porphyrin was developed. [Refs. 11, 18, 19]

### **Interaction of organic-inorganic matrices with immobilized biological material**

(G. Kuncová, supported by the MEYS, OC COST project No. OC121)

Monitoring of natural fluorescence of living cells and production of coloured intermediates were used for determination of yeast viability and construction of whole cell optical sensors of polychlorinated biphenyls. [Ref. 1, 6, 9]

### **Polymeric antidegradants based on liquid polybutadienes, polysiloxanes and their block copolymers**

(J. Heflejš, joint project with IMC, SYNPO Pardubice, and UPa, supported by GA CR, grant No. GA203/07/0987)

The research has been focused on the synthesis of N-containing antidegradants immobilized on poly(siloxanes) containing terminal hydroxylalkyl groups. Alternative protocols for the synthesis of these novel compounds were worked out. The hydroxyalkyl substitution of these antidegradants enables their immobilization by incorporation into polyurethane matrix during polymer preparation.

**Monitoring and remediation of environmental pollution with advanced organic-inorganic materials – MOREPIM**

(G. Kuncová, supported by MEYS, KONTAKT project No. ME 892)

The aim of the project is application of novel materials, developed in Oak Ridge National Laboratories (ORNL), in construction of optical sensors and in remediation processes, which are investigated in ICPF. The research will cover utilization of inorganic and organic-inorganic nanoparticles in design of sensors for monitoring of biotechnological processes and preparation of novel immobilized biocatalysts. [Ref. 12]

**Whole cell optical sensors (WOCOS)**

(G. Kuncová, supported by MEYS, KONTAKT project No. ME 893)

The aim of the project is novel whole-cell optical sensor for continual monitoring of pollution in remote localities, which will be equipped with both chemical and biological transducers. The optical fiber sensor should be used for early warning detection of toxic pollution and bioavailability of contaminants which might be removed by biodegradation. [Ref. 17]

**Enzymatically catalyzed synthesis of alkyd resins (ENZALKYD)**

(G. Kuncová, joint project with SYNPO Pardubice, supported by MIT, project No. MPO 2A-3TP1/108)

The project is aimed at application of regioselective lipase type enzyme catalysts in the first step of alkyd resin synthesis, so called alcoholysis, which is based on reesterification of vegetable oils with low molecular weight polyols.

**Optical chemical sensors - OPTISENS**

(G. Kuncová joint project with University of Maribor, Slovenia, supported by MEYS, KONTAKT project No. MEB 090817)

The aim of the project is preparation of sensitive elements of optical sensors and application of these in the packing of poultry meat and evaluation of their utility for control of freshness of packed meat.

**International co-operations**

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

Center for Environmental Biotechnology University of Tennessee, USA: Improved biomaterials for the encapsulation of living cells

Environmental Sciences Division Oak Ridge National Laboratories, Oak Ridge TN, USA: Application of nanomaterials and novel organic-inorganic materials in optical sensors

Centro de Engenharia Biológica, Universidade do Minho, Braga, Portugal: Monitoring of viability of immobilized cells by optical methods

Universidade Nova de Lisboa, Lisbon: Immobilization of lipase and cutinase on inorganic supports

## Teaching

F. Kaštánek: ICT, course "Bioengineering"

J. Čermák: UJEP, courses "Organic chemistry I" and "Organic chemistry II"

## Publications

### Original papers

1. Gavlasová P., Kuncová G., Kochánková L., Macková M.: Whole Cell Biosensor for Polychlorinated Biphenyl Analysis Based on Optical Detection. *Int. Biodeterior. Biodegrad.* 62(3), 304-312 (2008).
2. Klusoň P., Drobek M., Strašák T., Kalaji A.: Photoinduced Catalytic Partial Oxidation of Citronellol with Assistance of PHCs. *React. Kinet. Catal. Lett.* 95(2), 231-238 (2008).
3. Pošta M., Čermák Jan, Sýkora J., Vojtíšek P., Císařová I., Fajgar R.: Square-planar Diphosphinoazine Rhodium(I) Amido Carbonyl Complexes with an Unsymmetrical PNP' Pincer-type Coordination. *J. Organomet. Chem.* 693(11), 1997-2003 (2008).
4. Slavětínská L., Mosinger J., Dračínský M., Pošta M.: NMR Study of Host-Guest Complexes of Disulfonated Derivatives of 9, 10-Diphenylanthracene and Corresponding Endoperoxides with Cyclodextrins. *J. Incl. Phenom. Macrocycl. Chem.* 61(3-4), 241-250 (2008).
5. Storch J., Čermák Jan, Pošta M., Sýkora J., Císařová I.: Palladium(II) Aryl-amido Complexes of Diphosphinoazines in Unsymmetrical PNP' Pincer-type Configuration. *J. Organomet. Chem.* 693(18), 3029-3034 (2008).
6. Šabata S., Lehnert R., Karban J., Hetflejš J., Kuncová G.: Dekontaminace podzemní vody obsahující terc-butylmethyleter a aromatické uhlovodíky fotolýzou peroxidu vodíku. (Czech) Decontamination of Ground Water Containing tert-Butyl Methyl Ether (MTBE) and Aromatic Compounds (BTEX) by Photolysis of H<sub>2</sub>O<sub>2</sub>. *Chem. Listy* 102(12), 1115-1120 (2008).
7. Kaštánek F., Kaštánek P., Maléterová Y.: Dechlorination of PCBs in Aqueous Mixtures with Zero-Valent Iron in Statu Nascendi. Influence of Microwaves on the Rate of Reaction. *J. Hazard. Mater.*, submitted.
8. Kaštánek P., Kaštánek F., Hájek M.: Microwave-enhanced Thermal Adsorption of Polyhalogenated Biphenyls from Contaminated Soil. *J. Hazard. Mater.*, submitted.
9. Kuřec M., Kuncová G., Brányik T.: Yeast Vitality Determination Based on Intracellular NAD(P)H Fluorescence Measurement during Aerobic-Anaerobic Transition. *Folia Microbiol.*, in press.
10. Pošta M., Čermák Jan, Vojtíšek P., Sýkora J., Císařová I.: Diphosphinoazine Rhodium(III) and Iridium(III) Octahedral Complexes. *Inorg. Chim. Acta*, in press.
11. Šabata S., Hetflejš J., Richtáriková R., Kuncová G., Lang K., Kubát P.: Immobilization of Porphyrins in Poly(hydroxymethylsiloxane). *Chem. Pap.*, in press.

### Chapters in books

12. Kuncová G.: Sensors with Biorecognition Elements Entrapped into Silica Based Polymers. In: *Sol-Gel Methods for Materials Processing*. (Plinio, I. - Zub, Y.L. - Kessler, V.G., Ed.), pp. 349-354, Springer, Dordrecht 2008.

## Patents

13. Storch J., Čermák Jan: Způsob přípravy racemických substituovaných helicenů. (Czech) Preparation of Racemic Substituted [6]Helicenes. Pat. No. PV 2008-831. Applied: 08.12.22.

## International conferences

14. Čermák Jan, Strašák T., Krupková A., Auerová K.: Alkene and Diene Complexes with  $[(C_5Me_4C_nF_{2n+1})Rh]$  Fragment for Fluorous Biphasic Catalysis. 16th International Symposium on Homogeneous Catalysis, ISHC-XVI, Book of Abstracts, p. P274, Florence, Italy, 06-11 July 2008.
15. Floriš T., Klusoň P., Bartek L., Storch J.: Quaternary Ammonium Salts as Reaction Media for Asymmetric Hydrogenation of beta-Ketoesters. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 215-221, Štrbské Pleso, Slovakia, 08-12 September 2008.
16. Kaštánek F., Kaštánek P., Maléterová Y.: Dechlorination of PCBs in Aqueous Mixtures with Zero-valent Nano-iron *In statu Nascendi*. Influence of Microwaves on the Rate of Reaction. 1st International Conference of Hazardous Waste Management, Book of Abstracts, p P25 (8 pp. full text on CD-ROM), Chania, Greece, 01-03 October 2008.
17. Kuncová G., Trögl J., Demnerová K., Ripp S., Sayler G.S.: Bioluminescent Bioreporters Encapsulated in Silica Gel. XVI International Conference on Bioencapsulation, Book of Abstracts, O08-2 - pp 1-4, Dublin, Ireland, 04-06 September 2008.
18. Kuncová G., Trögl J., Gavlasová P., Ripp S.A., Sayler G.S.: The Influence of Immobilization into Silica Sol-Gel Matrix on Response of Optical Whole-Cell Biosensors. 5th International Conference on SOL-GEL MATERIALS, Abstracts, p. 30, Trzebiezowice, Poland, 01-05 June 2008.
19. Rychtáriková R., Kuncová G., Krulikovská T., Sviráková E., Hetflejš J.: Biototoxicity Evaluation of Singlet Oxygen Generated by Immobilized Porphyrin. XVI International Conference on Bioencapsulation, Book of Abstracts, P19 - pp 1-4, Dublin, Ireland, 04-06 September 2008.
20. Sýkora J., Storch J., Karban J., Čermák Jan: Atropoisomerism of 1,8-bis-(2-Propynyl-phenyl)-naphthalene. International Conference on LC-NMR and Related Techniques: "Challenges in Biological Systems", Program - Abstract - Information, p. 20, Jena, Germany, 27-29 August 2008.

## Environmental Process Engineering Laboratory

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### Fields of research

- Persistent organic pollutants
- Fluidized bed combustion and gasification
- Gas-solid reactors and operations
- Gaseous and particulate emissions from combustion and industrial processes
- Solid waste treatment and co-combustion
- Preparation of the electrodeless discharge lamps for photochemical applications
- Investigation on the formation possibility of PCDD/F by synthetic reactions
- Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis

### Applied research

- Dechlorination of persistent organic pollutants
- Recovery of precious metals
- PET recycling
- Electronic scrap recycling
- Simultaneous disinfection and microwave drying of books and similar paper-based materials
- Microwave technology for production of new glasses
- Low-energy microwave depolymerization of waste poly(ethylene terephthalate) (PET) and polyurethane (PUR) foams

### Research projects

#### **Near zero emission advanced fluidised bed gasification (FLEXGAS)**

(M. Punčochář, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00005)

In this project, the ways are examined of overcoming the potential disadvantages of fluidised bed gasification, the technology for CO<sub>2</sub> capture/reduction and the advantages in terms of their ability to process biomass/waste in association with coal at different scales of operation and for different applications. [Refs. 5-7, 13, 14, 16-18, 24, 30, 39-41]

### **Phytoextraction biomass disposal – an unsolved problem**

(M. Punčochář, joint project with Czech University of Life Sciences, supported by GA CR, grant No. GA104/07/0977)

Potentially toxic elements such as Cd or Zn accumulated in the biomass of hyperaccumulating and/or highly accumulating plants are bound into different parts of the organic matrix in different extent and direct extraction of these elements is not straightforward. The aim of the project is to grow different plant species with the ability to accumulate metals in above ground biomass mainly willows and to develop procedure degrading organic matrix of the element accumulating plants, into the forms, where elements could be effectively extracted and recovered. [Refs. 29, 35-37, 43, 44]

### **Waste as raw material and energy source**

(M. Punčochář, joint project with Brno University of Technology, and EVECO Brno, supported by MEYS, project No. 2B08048)

The project is concerned with research and application of modern approaches leading to the higher effectivity in using different classes of wastes in energy and recycling processes. Attention is paid especially to the processes of thermal processing of wastes with aim of maximal use of produced energy with minimization of released harmful substances. The project involves both experiments and computer simulations. [Refs. 42, 43]

### **Fluidization and decontamination of organic-polluted solids in a fluid-bed reactor**

(M. Hartman, supported by ASCR, grant No. IAA400720701)

A fundamental understanding of such viable reaction systems for the thermal oxidation of organic liquids entrapped (absorbed) within porous solids is still lacking. The hydrodynamic behavior of the "g"-s suspensions with such polluted (wet and sticky) particles is explored with the aid of pressure fluctuations also with respect to their unwanted tendency to stick together and lie down. Hitherto unexplored, inert and porous particles soaked in model organic compounds will be fired in a bench-scale, fluid-bed reactor operated in different regimes. Experimental and modeling efforts seek to explain and describe the dependence of the reactor's combustion efficiency as a function of residence time, excess air, operating temperature and particle size. The study focuses on the overall picture of formation and oxidation destruction of main gaseous pollutants (NO, NO<sub>2</sub>, N<sub>2</sub>O, CO, organic residuals, persistent organic pollutants, SO<sub>2</sub>, and HCl) and their interrelationships. [Refs. 3, 10, 11, 15, 27]

### **Research of the production of hydrogen and synthesis gases by gasification of waste biomass originating from the production of biofuels**

(J. Hanika, V. Veselý, joint project with Research Institute of Inorganic Chemistry, Ústí n/L, supported by MIT, project No. 2A-2TP1/024)

Project is focused on gasification of waste biomass which comes from the production of bio-ethanol and bio-diesel. The aim is to produce hydrogen from biomass, to capture CO<sub>2</sub> rising in the process and to separate present heteroatoms. A specific task of project is to develop the integral process which includes the processing of biomass into existing technology of waste crude oil gasification. [Ref. 45]

**PETELYSE-PET recycling**

(V. Veselý, joint project with ICT, supported by MIT, IMPULS project No. FI-IM4/096)

The technology of PET recycling developed in ICPF consists in PET flakes crystallization. Formed crystalline PET is crushed into small particles and then is subject to the basic hydrolysis at an atmospheric pressure. In addition to lye solution, glycol is added in the hydrolysis. Water is eliminated by boiling, which gives rise to suspension of sodium salt of terephthalic acid and glycol. The suspension is skimmed and the filtered glycol is vacuum distilled. Pure glycol is then the distillation product. Electrolysis removes pure terephthalic acid salt from the solution. Glycol solution is returned to the hydrolysis. Terephthalic acid is precipitated by a mineral acid. Terephthalic acid and glycol are products in a "polymer grade" quality. The waste is a part of washing waters, distillation remainders after glycol regeneration and a filter cake after the terephthalate solution filtration. The main aim of the project is to produce reliable data for scaling up of the process and to evaluate the economy of whole recycling. [Refs. 22, 47, 48]

**New technologies for recovery of precious and special metals from electrical and electrotechnical wastes**

(V. Gruber, joint project with SAFINA, supported by MIT, IMPULS project No. FI-IMS/075)

The project deals with recovery of precious metals from electrical and electrotechnical wastes. Special attention is paid to the recovery of Eu and Y from TV sets. [Ref. 25]

**Preparation of the electrodeless discharge lamps for photochemical applications**

(V. Církva, supported by GA CR, grant No. GA104/06/0992)

The project is concerning on preparation of the electrodeless discharge lamps (EDLs) as a suitable source of UV/VIS light for photochemical reactions. The EDL consists of a glass tube filled under a lower pressure with an inert gas and an excitable substance (mercury, sulfur), and generates UV/vis radiation when placed into the microwave field. The effect of operating EDL parameters, the microwave power output and medium properties on spectral characteristics are studied. [Refs. 2, 20, 49, 50, 51]

**Investigation on the formation possibility of PCDD/F by synthetic reactions from their surrogates**

(V. Církva, supported by GA CR, grant No. GA104/07/1212)

The project is directed toward a study of the synthetic reactions producing persistent organic pollutants of the type of PCDD and PCDF, with special emphasis on the conditions of formation of these substances in combustion plants. Investigation is focused on the formation possibility of PCDD/F from their surrogates. As the major proposed surrogates are chlorinated phenols and benzenes. The research is also oriented on the formation study of new PCDD/F intermediates and precursors on suitable solid supports from corresponding surrogates. Attention is paid to the effects of matrices and of copper metal forms with various physico-chemical properties on the course of the synthetic reactions. The research results should contribute to initiation of further technical measures in combustion plants that would decrease PCDD/F emissions. [Refs. 1, 8, 9, 32, 33, 42]

**Optimization of offgas cleaning system with safe and reliable dioxin destruction**

(V. Pekárek, supported by MEYS, project No. OE 200)

The application of the original Czech CMD detoxification technology was solved for the supplementation of the REMEDIA catalytic filter (Gore) in the Czech municipal waste incineration plant TERMIZO, Inc. The organic persistent compounds (POPs) in the fly ashes

were detoxified at least from 98% at 350 °C by the CMD technology. By this way the incineration plant might be supposed for POPs compounds as wasteless. The CMD technology was successfully proved in semi industrial scale. The detoxification ability was tested by using different matrices for different POPs compounds. [Refs. 1, 4, 28, 32, 33]

### **Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis**

(M. Hájek, supported by GA CR, grant No. GA104/08/0416)

The research has been focused on application in heterogeneously catalyzed reactions in liquid phase. It has been observed that selectivity of catalytic reaction can be significantly improved. These important findings evoked continuation to study this effect in more detail, what is the subject of this project. Scope and limitation of this method including possibility of potential applications has been studied on model reactions with non-polar (non-absorbing) reactants (alkylation of aromatics by alkenes) in the presence of strong acidic (strong absorbing) solid catalysts. [Refs. 12, 26, 38]

### **Simultaneous disinfection and microwave drying of books and similar paper-based materials**

(M. Hájek, supported by ICPF)

New technology for drying of flooded books including simultaneous disinfection has been completed and protected by EP patent. [Ref. 19]

### **Microwave technology for production of new glasses**

(M. Hájek, J. Brustman, supported by ICPF)

Production of new glasses by microwave radiation has been developed obtaining better properties compared to conventional melting process. [Ref. 31]

### **Low-energy microwave depolymerization of waste poly(ethylene terephthalate) (PET) and polyurethane (PUR) foams**

(M. Hájek, J. Sobek, supported by ICPF)

Microwave energy is applied for total depolymerization of waste PET material, especially waste PET bottles. The products are terephthalic acid and ethylene glycol. The process includes the following steps: depolymerization, purification and separation. Total depolymerization is achieved by applying microwave energy of 2450 MHz frequency with energy consumption of 0.5-1.0 kWh/kg PET. A developed recycling process is based on the chemolysis of polyurethane (PUR) foams using proper diols or triols in combination with microwaves heating. The product is a liquid recyclate with active hydroxyl groups. [Ref. 21]

### **Cooperation of EPEL with Prague City Hall**

(V. Tydlitát, supported by Prague City Hall, department Protection of Environment)

Dependences of polycyclic aromatic hydrocarbons (PAHs) concentration in Prague atmosphere on mean atmosphere temperature in years 2006 and 2007 are presented and discussed. [Ref. 46]

### **Emission factors of POPs and heavy metals from small sources**

(V. Pekárek, joint project with TU Ostrava, supported by MEYS, project No. SP/1a2/116/07)

Determination of emission factor for selected POPs compounds and heavy metals is solved. The following topics will be studied (i) the validation of the original air dilution unit for the sampling, (ii) effect of different combustion units from the standpoint of toxic compounds emission, (iii) effect of different fuels on the toxic compounds formation. [Ref. 4]



## International co-operations

Vienna University of Technology, Vienna, Austria: Gasification

Croucher Institute for Environmental Sciences, Hong Kong, Baptist University: Phytoextraction

Institute for Energy, Joint Research Centre, Petten, The Netherlands: Pressurized fluidized bed combustion/gasification technologies; Waste incineration/gasification

University of KwaZulu-Natal, Durban, Republic of South Africa: Gaseous and particulate emissions

## Teaching

M. Punčochář, P. Kameníková, M. Pohořelý and M. Vosecký: Czech University of Life Sciences Prague, course "Renewable and alternative sources of energy"

## Publications

### Original papers

1. Bureš M., Pekárek V., Ocelka T.: Thermochemical Properties and Relative Stability of Polychlorinated Biphenyls. *Environ. Toxicol. Phar.* 25(2), 148-155 (2008).
2. Církva V., Žabová H., Hájek M.: Microwave Photocatalysis of Mono-Chloroacetic Acid over Nanoporous Titanium(IV) Oxide Thin Films Using Mercury Electrodeless Discharge Lamps. *J. Photochem. Photobiol., A* 198(1), 13-17 (2008).
3. Hartman M., Trnka O.: Physical Characteristics of Fluidized Beds via Pressure Fluctuation Analysis. *AIChE J.* 54(7), 1761-1769 (2008).
4. Horák J., Hopan F., Krpec K., Dej M., Machálek P., Pekárek V., Šyc M., Ocelka T., Tomšej T.: Emise POP a těžkých kovů z malých zdrojů znečišťování a jejich emisní faktory. (Czech) POPs and Heavy Metal Emissions from Small Sources and Their Emission Factors. *Ochrana ovzduší* 21(56), 38-41 (2008).
5. Kalisz S., Svoboda K., Robak Z., Baxter D., Andersen L.K.: Application of FT-IR Absorption Spectroscopy to Characterize Waste and Bio-Fuels for Pyrolysis and Gasification. *Arch. Waste Management Environ. Protect.* 8, 51-62 (2008).
6. Miccio F., Kalisz S., Baxter D., Svoboda K.: Combustion of Liquid Bio-Fuels in an Internal Circulating Fluidized Bed. *Chem. Eng. J.* 143(1-3), 172-179 (2008).
7. Miccio F., Svoboda K., Schosger J.-P., Baxter D.: Biomass Gasification in Internal Circulating Fluidized Beds: A Thermodynamic Predictive Tool. *Korean J. Chem. Eng.* 25(4), 721-726 (2008).
8. Slavětínská L., Mosinger J., Dračinský M., Pošta M.: NMR Study of Host-Guest Complexes of Disulfonated Derivatives of 9,10-Diphenylanthracene and Corresponding Endoperoxides with Cyclodextrins. *J. Incl. Phenom. Macrocycl. Chem.* 61(3-4), 241-250 (2008).
9. Slavětínská L., Mosinger J., Kubát P.: Supramolecular Carriers of Singlet Oxygen: Photosensitized Formation and Thermal Decomposition of Endoperoxides in the Presence of Cyclodextrins. *J. Photochem. Photobiol., A* 195(1), 1-9 (2008).

10. Hartman M., Trnka O.: Drag Coefficients from Explicit Relationships for the Terminal Fall Velocity of Spheres. Chem. Eng. Sci., submitted.
11. Hartman M., Trnka O.: Monitoring the Fluidization Behavior through Time Series of Pressure Fluctuations in a Bed. AIChE J., submitted.
12. Kaštánek P., Kaštánek F., Hájek M.: Microwave-enhanced Thermal Adsorption of Polyhalogenated Biphenyls from Contaminated Soil. J. Hazard. Mater., submitted.
13. Martinec J., Šen H., Svoboda K., Martinčová J.V., Baxter D.: The Thermal Protection of a Specific Experimental Instrument for Monitoring of Combustion Conditions on the Grate of Municipal Solid Waste Incinerators. Appl. Therm. Eng., submitted.
14. Svoboda K., Wieczorek K., Miccio F., Baxter D., Kalisz S.: Simplified Modeling of Circulating Flow of Solids between a Fluidized Bed and a Vertical Pneumatic Transport Tube Reactor Connected by Orifices. Powder Technol., in press.

#### Review papers

15. Hartman M., Trnka O.: Těžké kovy v čistírenském kalu a jejich chování při spalování. (Czech) Heavy Metals in Sewage Sludge and Their Behaviour in Incineration. Chem. Listy 102(2), 131-138 (2008).
16. Svoboda K., Siewiorek A, Baxter D., Rogut J., Pohořelý M.: Thermodynamic Possibilities and Constraints for Pure Hydrogen Production by a Nickel and Cobalt-Based Chemical Looping Process at Lower Temperatures. Energ. Convers. Manage. 49(2), 221-231 (2008).
17. Svoboda K., Pohořelý M., Hartman M., Martinec J.: Pretreatment and Feeding of Biomass for Pressurized Entrained Flow Gasification. Fuel Process. Technol., submitted.
18. Svoboda K., Pohořelý M., Martinec J., Baxter D.: Integration of Biomass Drying with Combustion/Gasification Technologies and Minimization of Emissions of Organic Compounds. Bioresource Technol., in press.

#### Patents

19. Hájek M., Drahoš J.: Method of Drying of Book and Similar Paper Material and Equipment for Its Processing. Pat. No. EP 1441191. Applied: 22.12.2003, Granted: 08.02.13.
20. Žabová H., Círka V., Hájek M.: Zařízení k provádění fotokatalytických reakcí. (Czech) Equipment for Photocatalytic Reactions. Pat. No. PUV 2007-19451/UV 18240. Applied: 07.11.30, Granted: 08.02.05.
21. Hájek M., Sobek J., Brustman J.: Method for the Chemical Depolymerization of Waste Polyethylene Terephthalate. Pat. No. PCT/EP/2008/058917. Applied: 08.07.09.
22. Novák L., Černín A., Hanika J., Veselý V.: Způsob a zařízení pro izolaci kyseliny tereftalové. (Czech) Princip and Device for Terephthalic Acid Isolation. Pat. No. PV 2008-602. Applied: 08.10.09.
23. Punčochář M., Skoblia S., Kameníková P.: Způsob stanovení celkového obsahu dehtu v plynu produkovaném zplyňováním paliva. (Czech) Method of Total Tar Content Determination in Gasifier Gas. Pat. No. PV 2008-780. Applied: 08.12.08.
24. Tydlitát V.: Laboratorní přehřívač vodní páry. (Czech) Laboratory Steam Overheater. Pat. No. PUV 2008-19643/UV18380. Applied: 08.02.04, Granted: 08.03.17.

## International conferences

25. Gruber V.: Recovery of Yttrium and Europium from Waste Luminophors from Spent CRT Displays. Pollutec 2008, Workshop Proceedings, pp. 1-3, Lyon, France, 02-05 December 2008.
26. Hájek M.: Application of Microwave Effects in Heterogeneous Catalysis. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 21-27, Štrbské Pleso, Slovakia, 08-12 September 2008.
27. Hartman M., Trnka O., Svoboda K.: Pressure Fluctuations in a Gas-Solid Fluidized Bed. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 140 (11 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
28. Horák J., Hopan F., Krpec K., Dej M., Kubačka M., Pekárek V., Šyc M., Ocelka T., Tomšej T., Machálek P.: Determination of Emission Factors for Combusting Solid Fuels in Residential Combustion Appliances. 28th International Symposium on Halogenated Persistent Organic Pollutants-Dioxin 2008, Organohalogen Compounds, Vol. 70, pp. 2470-2473, Birmingham, Great Britain, 17-22 August 2008.
29. Jeremiáš M., Pohořelý M., Vosecký M., Skoblia S., Kameníková P., Svoboda K., Punčochář M.: Alotermní fluidní zplyňování biomasy. (Czech) Alotermal Fluidized Bed Biomass Gasification. 7. mezinárodní konference Chemie energetických cyklů, Sborník přednášek, pp. 107-115, Praha, Czech Republic, 09-10 September 2008.
30. Martinec J., Svoboda K., Martincová J.V.: Monitoring and Evaluation of the Incineration Process on the Moving Grate in Municipal Solid Waste Incinerators. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 150 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
31. Matějková A., Hájek J., Hájek M.: Metoda tavení skla pomocí mikrovlnné energie, nové možnosti odlévání skleněných soch a plastik. (Czech) The Method of Glass Melting by Microwave Energy, New Possibilities of Casting Glass Sculpture. Česká a Slovenská konference o skle, Sborník příspěvků, Sklář a keramik, ročník 58 C, pp. 21-24, Luhačovice, Czech Republic, 05-07 November 2008.
32. Ocelka T., Grabic R., Církva V., Šyc M., Kodeš V., Leontovyčová D., Pekárek V.: Contamination of Czech Rivers and Dreissena Polymorpha with PCBs from the Point of View of the Ortho Side Chlorinated Congeners. 28th International Symposium on Halogenated Persistent Organic Pollutants-Dioxin 2008, Organohalogen Compounds, Vol. 70, pp. 002001-002004, Birmingham, Great Britain, 17-22 August 2008.
33. Ocelka T., Pekárek V., Sekula P.: Technology for POPs Destruction: Copper Mediated Destruction (CMD). Contaminated Sites Bratislava 2008, Conference Proceedings, pp. 182-183, Bratislava, Slovakia, 10-13 July 2008.
34. Pekárek V.: 30letá historie kalorimetrických seminářů. (Czech) 30 Years' History off Calorimetric Meetings. 30 Mezinárodní český a slovenský kalorimetrický seminář, Sborník příspěvků, pp. 11-16, Rožnov pod Radhoštěm, Czech Republic, 26-30 May 2008.
35. Pohořelý M., Šyc M., Tlustoš P., Habart J., Punčochář M.: Vyluhovatelnost Zn, Cd, Pb a Cu ze vzorku penízku modravého (*Thlaspi caerulescens*) použitého pro fytoremediaci. (Czech) Leaching of Zn, Cd, Pb, a Cu from Penny-Cress (*Thlaspi caerulescens*) Used for Phytoremediation. 17. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, p. 2390-2395, Milovy, Czech Republic, 14-16 April 2008.
36. Punčochář M., Šyc M., Pohořelý M., Habart J., Tlustoš P.: Postharvest Processes of Biomass Contaminated by Heavy Metals. 14th International Conference on Heavy

- Metals in the Environment, Proceedings , pp. 532-534, Taipei, Taiwan, 16-23 November 2008.
37. Punčochář M., Šyc M., Pohořelý M., Tlustoš P.: Methods of Treatment of Contaminated Biomass from Heavy Metals Phytoremediation. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 113, Tatranské Matliare, Slovakia, 26-30 May 2008.
  38. Sobek J., Hájek M.: Alkylation of Aromatics by Alkenes in the Microwave Field. 9th Pannonian International Symposium on Catalysis, Book of Abstracts, pp. 453-458, Štrbské Pleso, Slovakia, 08-12 September 2008.
  39. Svoboda K., Baxter D., Miccio F., Kalisz S., Pohořelý M.: Simplified Modeling of Circulating Flow of Solids between a Fluidized Bed and a Vertical Pneumatic Transport Tube Reactor Connected by Orifices. BIOGASTECH, Book of Abstracts, pp. 1-21, Gebze, Turkey, 09-11 April 2008.
  40. Svoboda K., Kalisz S., Martinec J., Pohořelý M.: Gas Bypassing and Circulation of Sand and Char Particles in a Dual System with Fluidized Bed and Pneumatic Transport – Effects of Design and Operation Parameters. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 3, p. 955 (16 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
  41. Svoboda K., Pohořelý M., Hartman M., Trnka O.: Pretreatment and Feeding of Biomass for Pressurized Entrained Flow Gasification. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 227 (14 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
  42. Šyc M., Pekárek V., Fišerová E., Karban J., Punčochář M.: The Effect of MSWI Start-up and Shut-down on Congener Profiles of PCDD/F Precursors. 28th International Symposium on Halogenated Persistent Organic Pollutants-Dioxin 2008, Organohalogen Compounds, Vol. 70, pp. 001810-001813, Birmingham, Great Britain, 17-22 August 2008.
  43. Šyc M., Pohořelý M., Toufarová H., Žáčková P., Punčochář M.: Palivářská charakteristika lnu setého použitého k fytoremediaci znečištěných průmyslových oblastí. (Czech) Fuel Characteristics of Flax (*Linum usitatissimum*) Applied for Phytoremediation of Industrially Contaminated Sites. 17. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, pp. 2396-2400, Milovy, Czech Republic, 14-16 April 2008.
  44. Tlustoš P., Szaková J., Habart J., Pavlíková D., Punčochář M., Najmanová J.: Comparison of Pot and Field Growing Conditions for the Cadmium and Zinc Accumulation by Plants Grown at Contaminated Soils. 14th International Conference on Heavy Metals in the Environment, Proceedings , pp. 182-185, Taipei, Taiwan, 16-23 November 2008.
  45. Tukač V., Hanika J., Veselý V., Lederer J., Nečesaný V.: Termodynamický rozbor parciální oxidace bioodpadu a rafinerských zbytků. (Czech) Thermodynamics of Biowaste and Refinery Waste Partial Oxidation. 17. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, p. 1174-1181, Milovy, Czech Republic, 14-16 April 2008.
  46. Tydlitát V., Kotlík B., Janota J.: Polycyklické aromatické uhlovodíky v pražské atmosféře během let 2006 a 2007. (Czech) Polycyclic Aromatic Hydrocarbons in the Prague Atmosphere during the Years 2006 and 2007. IX. konference České aerosolové společnosti, Sborník konference, pp. 47-50, Praha, Czech Republic, 04 December 2008.
  47. Veselý V., Hanika J.: PET Bottles Recycling. Pollutec 2008, Workshop Proceedings, pp. 1-6, Lyon, France, 02-05 December 2008.

48. Veselý V., Hanika J., Čech B.: Nová metoda chemické recyklace PET lahví. (Czech) A New Method of PET Botles Chemical Recycling. 60. Jubilejní sjezd asociací českých a slovenských chemických společností, Chemické Listy 102(8), p. 648, Olomouc, Czech Republic, 01-04 September 2008.
49. Žabová H., Církva V.: Photocatalytic Reactions in a Microwave Fields Using an Electrodeless Discharge Lamp. 60. Jubilejní sjezd asociací českých a slovenských chemických společností, Chemické Listy 102(8), p. 630, Olomouc, Czech Republic, 01-04 September 2008.
50. Žabová H., Církva V.: The Electrodeless Discharge Lamps Coated with the Titania Thin Film for Photocatalysis in a Microwave Field. XXII IUPAC Symposium on Photochemistry 2008, Abstracts, p. 257, Gothenburg, Sweeden, 28 July - 01 August 2008.
51. Žabová H., Církva V.: Visible-Light Active Titanium Dioxide for Microwave Assisted Photocatalytic Reactions Using Electrodeless Discharge Lamp. The 4th International Conference on Technological Advances of Thin Films 2008 and Surface Coatings, Book of Abstracts, p. 212 (ID-4069), Singapore, Singapore, 13-16 July 2008.

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### Fields of research

- Composition, size and hygroscopicity 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
- Combustion aerosols
- Emissions sampling

### Research projects

#### European supersites for atmospheric aerosol research

(J. Smolík, supported by EC, project No. FP6-026140-EUSAAR)

European infrastructure project EUSAAR is focused on improving the current state of aerosol measurement on European supersites for atmospheric aerosol measurement. This aim is being reached by dissemination of knowledge from basic technical level to setting-up a state of the art of experimental methods on selected sites. QA/QC procedures, intercalibration of both basic and advanced measurement methods together with development of new aerosol instrumentation are the ways to fulfill the aims of the project. [Refs. 16, 37]

#### European integrated project on aerosol cloud climate and air quality interactions

(J. Smolík, supported by EC, project No. FP6-036833-2-EUCAARI)

European infrastructure project EUCAARI is designed as a research chain that aims to advance our understanding of climate and air quality through a series of connected activities beginning at the molecular scale and finishing at the regional and global scale. EUCAARI will build upon the pool of available data from previous field campaigns and long-term measurements in order to establish globally consistent data sets. A hierarchy of complementary models, at the molecular, process, meso-, regional and the global scale will be applied in a coordinated way in EUCAARI.

**Improvement of the assessment methods of ambient air pollution loads of PM<sub>10</sub> in the Czech Republic**

(J. Smolík, joint project with Czech Hydrometeorological Institute and Norwegian Institute for Air Research, supported by Norwegian Funds (via Ministry of Finance of CR), project No. CZ 0049)

The aim of the project is to improve the characterization of PM<sub>10</sub> suspended particles with the focus on secondary particle contribution, proposal of chemical model of secondary particles formation, identification of sources, and application and verification of dispersion models. The project provides direct support to the improvement of ambient air quality in the Czech Republic, respects the principle of air pollution prevention and meets the conception of sustainable development. [Refs. 41-43]

**Evaluation of dynamics of aerosol particles in indoor environment**

(J. Smolík, joint project with CTU, supported by GA CR, grant No. GA101/07/1361)

The aim of the proposed project is to study experimentally the behaviour of aerosol particles in three different indoor environments: a full-scale laboratory room, unfurnished room in an apartment, and whole furnished apartment and to compare experimental results with theoretical predictions according to zonal mass-balance (MC-SIAM) and CFD (Fluent/FPM) modelling. The measurements will be done both under well-defined laboratory conditions (simple geometry, defined indoor boundary conditions, laboratory generated aerosol with narrow size distribution) and "real" condition (furnished and/or unfurnished rooms, aerosol from different typical activities indoors, air exchange between indoor and outdoor environment and between compartments indoors). The purpose of the study is to test applicability of zonal mass-balance and CFD modelling and simulation for the prediction of indoor aerosol dynamics. [Refs. 17, 18, 38-40]

**Particulate matter: Properties related to health effects**

(J. Smolík, supported by ESF, COST Action 633)

The project focuses on the development and evaluation of scientific methodologies and databases that would improve the scientific understanding and regulatory basis on the physico-chemical constituents and emission sources of ambient air particulate matter causing the current substantial mortality and morbidity among European populations.

**Hygroscopic properties of urban and suburban carbonaceous aerosols**

(J. Schwarz, supported by MEYS, KONTAKT project No. ME 941)

The aim of this project is to study hygroscopic properties of real atmospheric aerosols in an urban environment. Cascade impactors with constant humidity sampling inlets (dry and wet) are going to be used to obtain size resolved samples. These samples are being analysed using ion chromatography in Prague and then for water soluble carbon in collaboration with Ghent University. This attitude aims to assess the influence of water soluble organic carbon on hygroscopicity of separated size fractions of urban aerosols. [Refs. 12, 46, 47]

**Composite nanoparticle synthesis by an aerosol process**

(P. Moravec, joint project with IIC and Tampere University of Technology, FI, supported by GA CR, grant No. GA104/07/1093)

Project involves an experimental study of nanoparticle synthesis by chemical vapour condensation method in an externally heated tube flow reactor. In the first part of the project: (i) single component metal and ceramic particles (Co, Ni, Pd, MnO) with great potential of applications will be prepared by thermal decomposition of corresponding metal-organic compounds. In the next step: (ii) binary mixed or coated metal-ceramic particles (TiO<sub>2</sub>-Co,

Al<sub>2</sub>O<sub>3</sub>-Ni, Al<sub>2</sub>O<sub>3</sub>-Pd) with potential use as catalyst and binary metal-ceramic (Co-SiO<sub>2</sub>) and ceramic-ceramic (MnO-SiO<sub>2</sub>) particles with potential applications as gas sensors or in electronics will be prepared by simultaneous decomposition of two precursors. Particle morphology, crystallinity, and chemical composition will be examined by SEM, TEM, SAED, XRD, EDS, etc. Results obtained in a hot wall reactor will be compared with those from experiments with liquid flame spray reactor at Tampere University of Technology. [Refs. 9, 27, 30, 33-35]

### **Friction materials based on polymer matrix containing metals and their impact on environment**

(P. Moravec, joint project with TU Ostrava and Southern Illinois University, USA, supported by GA CR, grant No. GA106/07/1436)

The project focuses on study of friction processes of laboratory prepared friction materials and original brake samples; further on structure identification of micro- and nanoscale wear particles with a view to reduce adverse anthropogenic impacts related to wear debris generation and deposition on the environment. An interdisciplinary and international CZE-US team consisting of researchers in the areas of materials science, chemistry, toxicology, medicine, and aerosol science will address the fundamental understanding of comprehensive material flow related to braking operations. The proposed research based on interconnection of material analyses and toxicological assessment (ecotoxicity, genotoxicity, and pulmonary toxicity) will allow identification of undesirable components in automotive friction materials and prediction of the environmental impact of wear particles release from brakes.

### **Influence of surface processes and electromagnetic radiation on transfer phenomena in aerosol systems with nanoparticles and porous bodies with nanopores**

(V.V. Levdanski, supported by GA AS CR, grant No. IAA400720804)

The aim of the proposed project is to perform a theoretical study of the influence of surface processes, size effects and electromagnetic radiation on transfer phenomena in aerosol systems with nanoparticles and in capillary-porous bodies with nanoscale pores taking into account physicochemical transformations on the particle and pore surface. It is assumed to study the joint influence of size effects, electric charge and adsorbable foreign gases on formation of nanoparticles. Novel methods of the membrane purification of gases under influence of resonance radiation are assumed to be considered. The effect of radiation on mass transfer and storage of hydrogen in metallic nanoparticles will be investigated. The influence of electromagnetic radiation on coagulation, coalescence of nanoparticles and their deposition on a surface will be studied. [Refs. 6-8, 10, 19, 27-33]

### **Determination of chemical and toxicological properties of suspended particles and study of their formation**

(J. Smolík, supported by Ministry of Environment, grant No. SP/1a3/148/08)

The aim of the proposed project is to suggest possible legal measures to decrease level of atmospheric aerosol burden in the Czech Republic. The sampling and chemical analysis of both particulate emissions and immissions at several types of sources and places in the Czech Republic, statistical analysis of the results and toxicological characterization of particles will be used to fulfill the aim of the project.



## International co-operations

- Philipps-University Marburg, Marburg, Germany: Experimental study of homogeneous nucleation in supersaturated vapours
- Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
- Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece: Urban aerosols. Modelling of transport processes in laminar diffusion cloud chamber: Comparison of methods determining atmospheric aerosol size distributions
- Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behaviour
- Technical University of Crete, Chania, Greece: Aerosols in the environment
- Tampere University of Technology, Tampere, Finland: Synthesis and characterisation of nanosized metal/ceramic particles
- Ghent University, Institute for Nuclear Sciences, Ghent, Belgium: OC/EC in urban and suburban PM10 aerosol in Prague, Hygroscopic properties of urban and suburban carbonaceous aerosols
- Southern Illinois University, Carbondale, USA: Friction materials based on polymer matrix containing metals and their impact on environment
- Division of Nuclear Physics, Department of Physics, Lund University, Lund, Sweden
- Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, Switzerland
- Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan
- Department of Chemical Engineering, Kongju National University, Korea

## Visits abroad

- L. Ondráčková: Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan (1 month)
- L. Štefancová: Ghent University, Institute for Nuclear Sciences, Ghent, Belgium (3 months)

## Visitors

- T. Hussein, University of Helsinki, Helsinki, Finland

## Teaching

- V. Ždímal: ICT, postgraduate course: "Aerosol Engineering"
- V. Ždímal: Faculty of Mathematics and Physics, CU, postgraduate course: "Aerosol Engineering"

## Publications

### Original papers

1. Brus D., Hyvärinen A.-P., Wedekind J., Viisanen Y., Kulmala M., Ždímal V., Smolík J., Lihavainen H.: The Homogeneous Nucleation of 1-Pentanol in a Laminar Flow Diffusion Chamber: The Effect of Pressure and Kind of Carrier Gas. *J. Chem. Phys.* 128(13), 134312-1-7 (2008).
2. Brus D., Ždímal V., Smolík J.: Homogeneous Nucleation Rate Measurements in Supersaturated Water Vapor. *J. Chem. Phys.* 129(17), 174501-8 (2008).
3. Hladil J., Strnad L., Šálek M., Jankovská V., Šimandl P., Schwarz J., Smolík J., Lisá L., Koptíková L., Rohovec J., Böhmová V., Langrová A.: An Anomalous Atmospheric Dust Deposition Event over Central Europe, 24 March 2007, and Fingerprinting of the SE Ukrainian Source. *Bull. Geosciences* 83(2), 175-206 (2008).
4. Karanasiou A., Eleftheriadis K., Vratolis S., Zarbas P., Mihalopoulos N., Mitsakou C., Housiadas C., Lazaridis M., Ondráček J., Džumbová L.: Size Distribution of Inorganic Species and Their Inhaled Dose in a Detergent Industrial. *Water, Air and Soil Pollution: Focus* 8(1), 71-76 (2008).
5. Lazaridis M., Džumbová L., Kopanakis I., Ondráček J., Glytsos T., Aleksandropoulou V., Voulgarakis A., Katsivela E., Mihalopoulos N., Eleftheriadis K.: PM10 and PM2.5 Levels in the Eastern Mediterranean (Akrotiri Research Station, Crete, Greece). *Water Air Soil Pollut.* 189(1-4), 85-101 (2008).
6. Levdansky V.V., Dragun V.L., Čížik S.A., Smolík J.: Vliyanie razmernykh effektov na koalestsentsiiu nanochastits. (Russ) *Vesti Nat. Ak. Nauk Belarusi, Ser. Fyz.-Tekh. Nauk* 3, 68-71 (2008).
7. Levdansky V.V., Smolík J., Moravec P.: Vliyanie razmernykh effektov na absorbtsiyu gaza nanochastsitsami. (Russ) *Inzh. - Fiz. Zh.* 81(5), 944-947 (2008).
8. Levdansky V.V., Smolík J., Moravec P.: Joint Effect of Particle Charge and Adsorbable Foreign Gases on Vapor Condensation on Fine Aerosol Particles. *Int. Commun. Heat Mass Transfer* 35(10), 1246-1248 (2008).
9. Levdansky V.V., Smolík J., Moravec P.: Effect of Surface Diffusion on Transfer Processes in Heterogeneous Systems. *Int. J. Heat Mass Transfer* 51(9-10), 2471-2481 (2008).
10. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Osobennosti fazovykh perekhodov pri formirovanii nanorazmernykh aerzolnykh chastits. (Russ) *Inzh. - Fiz. Zh. (J. Eng. Phys. Thermophys.* 81(2), 280-286) 81(2), 264-270 (2008).
11. Mitrakos D., Ždímal V., Brus D., Housiadas C.: Data Evaluation of Laminar Flow Diffusion Chamber Nucleation Experiments with Different Computational Methods. *J. Chem. Phys.* 129(5), 054503-1 - 7 (2008).
12. Schwarz J., Chi X., Maenhaut W., Civiš M., Hovorka J., Smolík J.: Elemental and Organic Carbon in Atmospheric Aerosols at Two Urban Background Sites in Prague. *Atmos. Res.* 99(2-4), 287-302 (2008).
13. Smolík J., Dohányosová P., Schwarz J., Ždímal V., Lazaridis M.: Characterization of Indoor and Outdoor Aerosols in Suburban Area of Prague. *Water Air Soil Pollut. Focus* 8(1), 35-47 (2008).
14. Večeřa Z., Mikuška P., Smolík J., Eleftheriadis K., Bryant Ch., Colbeck I., Lazaridis M.: Shipboard Measurements of Nitrogen Dioxide, Nitrous Acid, Nitric Acid and Ozone in the Eastern Mediterranean Sea. *Water Air Soil Pollut. Focus* 8(1), 117-125 (2008).

15. Wedekind J., Hyvarinen A.-P., Brus D., Reguera D.: Unraveling the "Pressure Effect" in Nucleation. *Phys. Rev. Lett.* 101(12), 125703 (2008).
16. Ždímal V., Brabec M., Wagner Z.: Comparison of Two Approaches to Modeling Atmospheric Aerosol Particle Size Distributions. *Aerosol Air Quality Res.* 8(4), 392-410 (2008).
17. Hussein T., Hruška A., Dohányosová P., Džumbová L., Hemerka J., Kulmala M., Smolík J.: Deposition Rates on Smooth Surfaces and Coagulation of Aerosol Particles Inside a Test Chamber. *Atmos. Environ.* 43(4), 905-914 (2009).
18. Hussein T., Kubincová L., Džumbová L., Hruška A., Dohányosová P., Hemerka J., Smolík J.: Deposition of Aerosol Particles on Rough Surfaces Inside a Test Chamber. *Build. Environ.*, in press.
19. Levdansky V.V., Smolík J., Moravec P.: Radiation-induced Mass Transfer through Membranes. *Int. Commun. Heat Mass Transfer*, in press.

#### International conferences

20. Brus D., Hyvärinen A.-P., Lihavainen H., Viisanen Y., Kulmala M.: Binary Homogenous Nucleation of Sulfuric Acid and Water Mixture. *European Aerosol Conference 2008, Book of Abstracts*, p. T03A036P, Thessaloniki, Greece, 24-29 August 2008.
21. Džumbová L., Smolík J.: Měření koncentrace aerosolových částic v barokním knihovním sále Národní knihovny. (Czech) Measurement of Aerosol Particles Concentration in Baroque Library Hall of National Library. IX.konference České aerosolové společnosti, *Sborník konference*, pp. 73-76, Praha, Czech Republic, 04 December 2008.
22. Hrubý J., Kolovratník M., Ždímal V., Jiříček I., Bartoš O., Moravec P.: Heterogeneous Particles in Steam Turbines: Measurements at Power Plant Prunéřov II and Further Development of Measuring Methods. IX. konference České aerosolové společnosti, *Sborník konference*, pp. 65-68, Praha, Czech Republic, 04 December 2008.
23. Chen S.C., Tsai C.J., Wu C.H., Chang C.S., Lin G.Y., Tsai J.H., Lin C.C., Chou Ch.C.K., Huang W.R., Roam G.D., Smolík J., Chen S.J.: Study of Environmental Nanoparticles at a Road Side and in a High-Way Tunnel. *European Aerosol Conference 2008, Book of Abstracts*, p. T04A014O, Thessaloniki, Greece, 24-29 August 2008.
24. Kolovratník M., Hrubý J., Ždímal V.: Částice v parních turbínách. (Czech) Particles in Steam Turbines. 7th Conference on Power System Engineering, Thermodynamics & Fluid Flow 2008, *Conference Proceedings*, pp. 69-72, Plzeň, Czech Republic, 26-27 June 2008.
25. Kolovratník M., Jiříček I., Hrubý J., Ždímal V.: Výzkum rozměrové struktury příměsí páry v turbínách. (Czech) Investigations on Size Structure of Steam Impurities in Turbines. 7. mezinárodní konference Chemie energetických cyklů, *Sborník přednášek*, pp. 158-161, Praha, Czech Republic, 09-10 September 2008.
26. Krejčí P., Ždímal V., Hrubý J., Schwarz J.: Measurement of Sulphuric Acid Vapour Pressure. *European Aerosol Conference 2008, Book of Abstracts*, p. T03A034P, Thessaloniki, Greece, 24-29 August 2008.
27. Levdansky V.V., Dragun V.L., Smolík J., Moravec P.: Tечение газов в наноразмерных капиллярах. (Russ) VI Minskii mezhnunarodnyi forum po teplo- i massoobmenu, *Tezisy dokladov i soobschenii*, p. 392, (7 pp. full text na CD-ROM), Minsk, Belarus, 19-23 May 2008.
28. Levdansky V.V., Smolík J., Moravec P.: Membrane Purification and Separation of Gases in Resonant Radiation Fields. *International Congress on Membranes and Membrane Processes, Poster Session Proceedings*, p. 119, Honolulu, Hawaii, USA, 12-18 July 2008.

29. Levdansky V.V., Smolík J., Moravec P.: Effect of Laser Radiation on Nanoparticle Formation by Deposition from Gas Mixture. European Materials Research Society, Abstracts, p. B-P1 10, Strasbourg, France, 26-30 May 2008.
30. Levdansky V.V., Smolík J., Moravec P.: Vliyanie vozbuzhdeniya molekul vodoroda na evo massoperenos v metalicheskikh sistemakh. (Russ) VI Minskii mezhdunarodnyi forum po teplo- i massoobmenu, Tezisy dokladov i soobschenii, pp. 405-406, (8 pp. full text na CD-ROM), Minsk, Belarus, 19-23 May 2008.
31. Levdansky V.V., Smolík J., Moravec P.: Size Effect in Trapping of Atoms by Aerosol Nanoparticles. European Aerosol Conference 2008, Book of Abstracts, p. T03A053P, Thessaloniki, Greece, 24-29 August 2008.
32. Levdansky V.V., Smolík J., Moravec P.: Transfer Processes in Heterogeneous System under Effect of Resonance Radiation. International Conference Advanced Laser Technologies ALT'08, Book of Abstracts, Siófok, Hungary, 13-18 September 2008.
33. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Zakhvat molekul gaza nanochastitsami. (Russ) VI Minskii mezhdunarodnyi forum po teplo- i massoobmenu, Tezisy dokladov i soobschenii, p. 393, (8 pp. full text na CD-ROM), Minsk, Belarus, 19-23 May 2008.
34. Moravec P., Smolík J., Klementová M., Levdansky V.V.: MOCVD Nanoparticle Synthesis from Copper Acetylacetonate. European Aerosol Conference 2008, Book of Abstracts, p. T01A058P, Thessaloniki, Greece, 24-29 August 2008.
35. Moravec P., Smolík J., Klementová M., Levdansky V.V.: CuO<sub>x</sub> Nanoparticle Production from Copper Acetylacetonate. IX. konference České aerosolové společnosti, Sborník konference, pp. 59-62, Praha, Czech Republic, 04 December 2008.
36. Neitola K., Brus D., Sipilä M., Kulmala M.: Binary Homogeneous Nucleation of Sulfuric Acid-Water: Particle Size Distribution and Effect of Detector on Total Count and Determination of Critical Cluster Size. European Aerosol Conference 2008, Book of Abstracts, p. T03A041P, Thessaloniki, Greece, 24-29 August 2008.
37. Ondráček J., Dohányosová P., Ždímal V., Schwarz J., Krejčí P., Smolík J.: Nový typ HTDMA systému pro dlouhodobá měření hygroskopických vlastností atmosférických aerosolových částic. (Czech) New HTDMA System for Long Time Measurements of Hygroscopic Properties of Atmospheric Aerosol. IX. konference České aerosolové společnosti, Sborník konference, pp. 27-28, Praha, Czech Republic, 04 December 2008.
38. Ondráček J., Džumbová L., Stavová P., Ždímal V., Barták M., Smolík J.: Monodisperse Aerosol Particles in an Apartment. European Aerosol Conference 2008, Abstract, p. T10A012P, Thessaloniki, Greece, 24-29 August 2008.
39. Ondráček J., Džumbová L., Ždímal V., Stavová P., Barták M., Smolík J.: Behavior of Well Defined Aerosol Sources in a House. The 11th International Conference on Indoor Air Quality and Climate, Programme, p. 108, Copenhagen, Denmark, 17-22 August 2008.
40. Ondráček J., Džumbová L., Ždímal V., Šťávovalá P., Barták M., Smolík J.: Chování monodisperzních aerosolových částic v bytě – experimentální studie. (Czech) The Behavior of Monodisperse Aerosol Particles in a House - Experimental Study. IX. konference České aerosolové společnosti, Sborník konference, pp. 55-58, Praha, Czech Republic, 04 December 2008.
41. Římnáčová D., Ždímal V., Smolík J., Šilhavý J.: Vybrané výsledky z kontinuálního měření atmosférických aerosolů v Praze - Suchdole. (Czech) Selected Results of the Continuous Measurement of Atmospheric Aerosols in Prague – Suchdol. IX. konference České aerosolové společnosti, Sborník konference, pp. 31-36, Praha, Czech Republic, 04 December 2008.

42. Schwarz J., Štefancová L., Novák J., Macek V., Smolík J.: Composition of PM<sub>2.5</sub> in Prague during the Year 2006. European Aerosol Conference 2008, Book of Abstracts, p. T06A219P, Thessaloniki, Greece, 24-29 August 2008.
43. Schwarz J., Štefancová L., Novák J., Pokorný R., Smolík J.: Složení frakce PM<sub>2,5</sub> v Suchdole v roce 2006. (Czech) Chemical Composition of PM<sub>2,5</sub> at Suchdol in the Year 2006. IX. konference České aerosolové společnosti, Sborník konference, pp. 63-64, Praha, Czech Republic, 04 December 2008.
44. Schwarz J., Ždímal V., Řimnáčová D., Ondráček J., Ondráčková L., Havránek V., Smolík J., Bízek V.: Měření početních a hmotnostních velikostních distribucí v blízkosti dopravního zdroje (Jižní spojky). (Czech) Number and Mass Size Distribution Measurement Next to Traffic Source (Jizni spojka). IX. konference České aerosolové společnosti, Sborník konference, pp. 37-40, Praha, Czech Republic, 04 December 2008.
45. Stavová P., Ondráček J., Džumbová L., Barták M., Smolík J.: Airflow Measurements in a Two-Zone Apartment Using Two Tracer Gases. The 11th International Conference on Indoor Air Quality and Climate, Programme, p. 49 (8 pp. full text on CD-ROM), Copenhagen, Denmark, 17-22 August 2008.
46. Štefancová L., Schwarz J., Chi X., Maenhaut W., Ševčíková I., Smolík J.: Parallel Sampling of Urban Aerosol at Dry and Wet Conditions during Winter 2008. European Aerosol Conference 2008, Book of Abstracts, p. T06A200P, Thessaloniki, Greece, 24-29 August 2008.
47. Štefancová L., Schwarz J., Maenhaut W., Smolík J.: Theoretical Mass Size Distribution of Wet Particles Calculated from Ambient Aerosol Sampled upon Dry Conditions during Summer and Winter Campaign 2008. IX. konference České aerosolové společnosti, Sborník konference, pp. 29-30, Praha, Czech Republic, 04 December 2008.

## Laboratory of Laser Chemistry

Head: J. Pola  
Deputy: R. Fajgar  
Research staff: V. Dřínek, A. Galíková, J. Kupčík, D. Pokorná, M. Urbanová  
Part time: P. Stopka  
Technical staff: D. Bartlová  
PhD students: T. Křenek, V. Jandová

### Fields of research

- IR and UV laser induced chemistry
- IR and UV laser chemical vapour deposition of novel polymeric and Si-, Ge- and C-based materials
- IR laser-induced carbothermal reduction of oxides
- IR and UV laser photopolymerization in the gas phase
- UV laser chemical liquid deposition of metal nanosols and nanocomposites
- IR and UV laser induced ablation of polymers
- IR and UV laser deposition of TiO<sub>2</sub>-based photocatalysts

### Research projects

#### **New laser induced process for production of novel carbon-based nanomaterials and carbon-based nanomaterials with incorporated Si, N, and B heteroatoms**

(J. Pola, supported by ASCR, grant No. IAA400720619)

MW and GW UV laser-induced photolysis of gaseous benzene and acetylene has been demonstrated as a process leading to transient polyacetylenes and cumulenes and yielding nanostructured carbon soot whose properties depend on the precursor. Simultaneous back-side etching of silica adjacent to laser-induced plasma enables to enrich the soot with polyoxocarbosilane [Ref. 10]. This process with gaseous pyridine allows photochemical etching of silica and deposition of composites containing nanodomains of very rare chaoite in amorphous C/Si/O/N phase [Ref. 12]. Similar process conducted in solution with UV laser photolysis of Fe<sup>II</sup> acetylacetonate affords deposition of alpha-Fe/polyoxocarbosilane/carbon nanocomposite whose heating allows evolution to alpha-Fe<sub>2</sub>O<sub>3</sub>/Polyoxocarbosilane/Carbon Nanocomposite [Ref. 11]. IR laser thermal etching of silicon monoxide [Ref. 9] and silicon dioxide [Ref. 16] with carbonaceous decomposition products of benzene and acetylene leads to deposition of nanosized silicon oxycarbide (prepared for the first time) and Si/C/O/H phase. These processes occur through carbothermal reduction of silicon oxides.

**Pyrolytic and photolytic approach for the deposition of novel Si/Ge/C materials**

(V. Dřínek, joint project with JH IPC and IIC, supported by ASCR, grant No. IAA400720616)

A conventional pyrolysis of a novel precursor - tris(trimethylsilyl)germane at 300-400 °C was performed. It resulted in formation of Ge nanowires (NWs) enveloped in Si/C material. Structure of NWs consists of core (crystalline Ge), inner jacket (nanocrystalline Ge) and outer jacket (Si/C) as revealed by HRTEM analysis. In some NWs the core of hexagonal Ge was established. Further heating under vacuum to 900 °C led to a complete evaporation of Ge and yielded thin wall Si<sub>1-x</sub>C<sub>x</sub> nanotubes. Lengths of nanowires and nanotubes ranged up to several micrometers. Formation of such nanostructured material is strongly affected by using appropriate substrate and/or its processing prior deposition. [Refs. 1, 2, 5]

**Novel preparation and photocatalytic study of titania-based catalysts**

(R. Fajgar, supported by NATO collaborative project, project No. CBP.EAP.CLG.982078)

UV laser-induced deposition of TiO<sub>2</sub> and Ti/O/Si materials from TiCl<sub>4</sub>/O<sub>2</sub> (or TiCl<sub>4</sub>/SiCl<sub>4</sub>/O<sub>2</sub> mixtures) was studied. Prepared films, deposited on glass substrates were annealed up to 450 °C. Photocatalytic activity and hydrophilicity was studied. The films annealed to 350-400 °C possess good adhesion to glass substrate and revealed superhydrophilic properties. Deposition in the presence of chromyl chloride results in formation of chromium-doped films. The doped films were analyzed using available spectroscopic, microscopic and diffraction techniques and photocatalytic activity in the visible light was studied.

**Laser decomposition of cobalt and nickel carbonyls in the presence of acetylene for preparation of carbon encapsulated metal nanoparticles**

(R. Fajgar, joint project with JH IPC, IIC, and Institute of Physics of the ASCR, v.v.i., supported by GA CR, grant No. GA203/07/0546)

Mixture of iron pentacarbonyl, cobalt tricarbonyl nitrosyl and acetylene decomposes under UV laser irradiation to form CoFe alloy nanoparticles encapsulated in carbon. Minor products (benzene, vinylacetylene) are formed as a result of acetylene dimerization and trimerization. Analysis of the solid deposit confirmed formation of the amorphous CoFe nanoparticles with diameter 10 nm, encapsulated in the amorphous carbon. The heating of the deposit to 600, 900 and 1150 °C results in crystallization of CoFe as syn-wairauite and better encapsulation. Higher temperature (900 °C) causes crystallization of the carbon shells and formation of diamond layers, covering the CoFe nanocrystals. Magnetic measurements revealed strong superparamagnetic behaviour of the CoFe nanoparticles at temperatures up to 140 K.

**International co-operations**

Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodź, Poland: UV laser-induced crosslinking of polysiloxanes  
Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of nanosized metal chalcogenides and polycarbosilthianes  
National Institute of Advanced Industrial Research and Technology, Tsukuba, Japan: Laser control of organic reactions

- University of Crete, Heraklion, Greece: Laser induced chemical vapour deposition of polycarbosilthianes
- King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia: Laser degradation of contaminants in fuel oils
- National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania: Laser-induced CVD of Fe/polymer nanocomposites
- Faculty of Technology and Metallurgy, University of St. Cyril & Methodius, Skopje, R. Macedonia: Novel preparation and photocatalytic study of titania-based catalysts

## Visitors

- M.A. Alsunaidi, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia
- J. Blazevska-Gilev, University of St. Cyril & Methodius, Skopje, R. Macedonia
- L. Díaz, Instituto de Estructura de la Materia, CSIC, Madrid, Spain
- M. Marinkovski, University of St. Cyril & Methodius, Skopje, R. Macedonia
- R. Tomovska, University of St. Cyril & Methodius, Skopje, R. Macedonia

## Publications

### Original papers

1. Dřínek V., Galíková A., Šubrt J., Fajgar R.: Conventional Pyrolysis of  $[-C\equiv C-SiMe_2-C\equiv C-GeMe_2-]_n$  Polymer Precursor for Si/Ge/C Materials. *J. Anal. Appl. Pyrolysis* 81(2), 193-198 (2008).
2. Dřínek V., Šubrt J., Klementová M., Rieder M., Fajgar R.: From Shelled Ge Nanowires to SiC Nanotubes. *Nanotechnology* 20(3), 035606 (2008).
3. Galíková A., Pola J.: Highly Sensitive TGA Diagnosis of Thermal Behaviour of Laser-Deposited Materials. *Thermochim. Acta* 473(1-2), 54-60 (2008).
4. Gondal M.A., Masoudi H.M., Pola J.: Laser Photo-Oxidative Degradation of 4,6-Dimethyldibenzothiophene. *Chemosphere* 71(9), 1765-1768 (2008).
5. Klementová M., Rieder M., Dřínek V., Fajgar R., Šubrt J.: Structure of Coated Ge-nanowires. *Microsc., Microanal.* 14(Suppl. 2), 198-199 (2008).
6. Kowalewska A., Kupčík J., Pola J., Stanczyk W.A.: Laser Irradiation of Oligosiloxane Copolymer Thin Films Functionalized with Side Chain Bulky Carbosilane Moieties. *Polymer* 49(4), 857-866 (2008).
7. Minceva M., Fajgar R., Markovska L., Meshko V.: Comparative Study of  $Zn^{2+}$ ,  $Cd^{2+}$ , and  $Pb^{2+}$  Removal from Water Solution Using Natural Clinoptilolitic Zeolite and Commercial Granulated Activated Carbon. Equilibrium of Adsorption. *Sep. Sci. Technol.* 43(8), 2117-2143 (2008).
8. Ouchi A., Bastl Z., Boháček J., Šubrt J., Bakardjieva S., Bezdička P., Pola J.: Room-Temperature Reaction of Laser-Photolytically Generated Te Nanosols with Silver. *J. Photochem. Photobiol., A* 200(2-3), 187-191 (2008).
9. Pokorná D., Urbanová M., Šubrt J., Bastl Z., Pola J.: IR Laser-Induced Carbothermal Reduction of Silicon Monoxide. *J. Anal. Appl. Pyrolysis* 83(2), 180-184 (2008).



10. Pola J., Galíková A., Bastl Z., Vorlíček V., Bakardjieva S., Šubrt J., Ouchi A.: UV Laser Photolysis of 1,3-Butadiyne and Formation of a Polyoxocarbosilane-Doped Nanosized Carbon. *J. Photochem. Photobiol., A* 194(2-3), 200-205 (2008).
11. Pola J., Maryško M., Vorlíček V., Bakardjieva S., Šubrt J., Bastl Z., Ouchi A.: UV Laser Photolytic Solution Deposition of  $\alpha$ -Fe/Polyoxocarbosilane/Carbon Nanocomposite and Evolution to  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/Polyoxocarbosilane/Carbon Nanocomposite. *J. Photochem. Photobiol., A* 199(2-3), 156-164 (2008).
12. Pola J., Ouchi A., Bakardjieva S., Vorlíček V., Maryško M., Šubrt J., Bastl Z.: Laser Photochemical Etching of Silica: Nanodomains of Crystalline Chaoite and Silica in Amorphous C/Si/O/N Phase. *J. Phys. Chem. C* 112(34), 13281-13286 (2008).
13. Pola J., Pokorná D., Šubrt J., Papagiannakopoulos P.: IR Laser-Induced Co-Decomposition of Gaseous Trisilane and Carbon Disulfide. *J. Anal. Appl. Pyrolysis* 81(2), 231-236 (2008).
14. Pola J., Urbanová M., Santos M., Díaz L., Šubrt J.: IR Laser-Induced Co-Decomposition of Trisilane and Thiirane for Deposition of Polycarbosilthiane Films. *J. Anal. Appl. Pyrolysis* 81(2), 225-230 (2008).
15. Pošta M., Čermák Jan, Sýkora J., Vojtíšek P., Císařová I., Fajgar R.: Square-Planar Diphosphinoazine Rhodium(I) Amido Carbonyl Complexes with an Unsymmetrical PNP' Pincer-type Coordination. *J. Organomet. Chem.* 693(11), 1997-2003 (2008).
16. Urbanová M., Pokorná D., Bakardjieva S., Šubrt J., Bastl Z., Pola J.: IR Laser-Induced Carbothermal Reduction of Silica. *Eur. J. Inorg. Chem.* 2008(26), 4111-4116 (2008).
17. Blazevska-Gilev J., Bastl Z., Šubrt J., Stopka P., Pola J.: IR Laser Ablative Degradation of Poly(phenylene ether sulfone): Deposition of Films Containing Sulfone, Sulfoxide and Sulfide Groups. *Polym. Degrad. Stabil.* 94(2), 196-200 (2009).
18. Dřínek V., Vacek K.: IR Evidence of Peroxy Radical SiOO(.). *Appl. Phys. A: Solids Surf.*, submitted.

#### International conferences

19. Blazevska-Gilev J., Pola J.: IR Laser Ablation of Poly(acetate) Loaded with Metal Particles. 20th Congress of Chemists and Technologists of Macedonia, Abstract Book, p. 268, Ohrid, Macedonia, 17-20 September 2008.
20. Blazevska-Gilev J., Pola J.: IR Laser Ablation of Poly(vinyl chloride-co vinyl acetate). 20th Congress of Chemists and Technologists of Macedonia, Abstract Book, p. 270, Ohrid, Macedonia, 17-20 September 2008.
21. Dřínek V., Fajgar R., Klementová M., Šubrt J.: From Shelled Germanium Nanowires to SiC Nanotubes. 6th International Conference on Inorganic Materials, Poster Presentations, Dresden, Germany, 28-30 September 2008.
22. Galíková A., Pola J.: TGA: A Sensitive Diagnosis of Thermal Stability of Laser-Deposited Materials. 35th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 153 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 26-30 May 2008.
23. Klementová M., Dřínek V., Fajgar R., Šubrt J.: Structure of Coated Ge-nanowires. Microscopy and Microanalysis 2008, Book of Abstracts, Albuquerque, New Mexico, USA, 03-07 August 2008.
24. Tomovska R., Pola J.: ArF Laser Photolytic Deposition of Nanopolymeric Organosulfur Materials. 20th Congress of Chemists and Technologists of Macedonia, Abstract Book, pp. 57-58, Ohrid, Macedonia, 17-20 September 2008.

## Department of Analytical Chemistry

Head: J. Schraml  
Deputy: J. Horáček  
Research staff: M. Bártlová, V. Blechta, J. Karban, M. Kurfürst, E. Macháčková,  
L. Soukupová, J. Sýkora  
Technical staff: J. Lněničková, P. Cuřínová

### Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

### Applied research

- Development of new analytical methods
- Analytical services to the research departments of ICPF

### Research projects

#### Advanced techniques for $^{29}\text{Si}$ NMR spectroscopy

(J. Schraml, supported by GA CR, grant No. GA203/06/0738)

Two topics -  $^{29}\text{Si}$  -  $^{13}\text{C}$  spin-spin coupling constants and LC- $^{29}\text{Si}$ -NMR - are integrated under this project. The newly developed methods for measurements of the coupling constant and their relative signs [Ref. 1] enable otherwise difficult line assignments and comparison with theory [Ref. 7]. In the field of LC-NMR the aims of the project were already met in the previous year.

#### Reactivity of asymmetrically substituted epimino pyranoses

(J. Karban, point project with CU, supported by ASCR, grant No. IAA400720703)

Methods of fluorine introduction in the vicinity of the aziridine ring of 1,6-anhydro-2,3,4-trideoxy-2,3-epimino- $\beta$ -D-*ribo/lyxo*-pyranoses were studied. Cleavage of suitable dianhydro derivatives (carbohydrate epoxides) with  $\text{KHF}_2$  appears to be the most promising synthetic approach. An alternative approach utilizes cleavage of 3,4-aziridines with  $\text{F}^-$  on reaction with DAST followed by aziridine ring closure at positions 2,3. The study of the aziridine ring cleavage of 1,6-anhydro-2,3,4-trideoxy-2,3-tosylepimino- $\beta$ -D-*lyxo*-pyranose continued and revealed that the nucleophilic cleavage reactions provided products of both *trans*-diaxial and *trans*-diequatorial cleavage depending on the reaction condition and the nucleophile. Conformation and conformational flexibility of 1,6-anhydro-epiminohexopyranoses was

assessed by an X-ray analysis of a complete series of all configurational isomers of 2,3- and 3,4-aziridine derivatives [Ref. 9].

### **Structure of silyl moieties through $J(^{29}\text{Si}-^{13}\text{C})$ couplings as determined by triple $\{^1\text{H}, ^{13}\text{C}\}^{29}\text{Si}$ NMR experiment**

(J. Schraml, supported by ASCR, grant No. IAA400720706)

New methods for measurement of spin-spin couplings between  $^{29}\text{Si}$  and  $^{13}\text{C}$  nuclei in solutions utilize instrumental possibilities of triple resonance of  $^1\text{H}-^{13}\text{C}-^{29}\text{Si}$  nuclei which enhance the sensitivity to the extent that expensive isotopic enrichment, common for bio-NMR, is not needed [Ref. 11]. The developed methods were extended to  $^{15}\text{N}$  couplings [Ref. 4]. Using these experiments model series of compounds are measured and calculated [Ref. 8] to produce the dependence of the vicinal  $^{29}\text{Si}-^{13}\text{C}$  couplings on dihedral angles and, subsequently, also the dependence on the nature of substituents.

### **$^{29}\text{Si}$ -NMR structural analysis of branched organosilicon polymers and its application in LC-NMR**

(J. Kurfürst, supported by GACR, grant No. GP203/08/P412)

Project objective is to evolve generally applicable NMR method for structural analysis of branched siloxanes based on Si-Si connectivity. Besides the well-known methods, new pulse sequences employing gradient and shaped pulses will be developed. Experiments will be initially conducted on commercially available model compounds; in later phase of project series of models will be synthesized. The research will advance from simple linear and branched oligosiloxanes towards to more complex macromolecules. Simultaneously, developed methods will be adapted for HPLC analysis of organosilicon polymers and copolymers with  $^{29}\text{Si}$  NMR detection in stop-flow mode.

## **International co-operations**

Catholic University of Leuven, Leuven, Belgium: NMR in medicinal chemistry  
Technical University Graz, Austria:  $^{29}\text{Si}$  NMR

## **Teaching**

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

## **Publications**

Original papers

1. Blechta V., Schraml J.: Relative Signs of  $^{29}\text{Si}-^{13}\text{C}$  Couplings. *Magn. Reson. Chem.* 46(8), 734-738 (2008).
2. Kurfürst M., Kozmík V., Svoboda J., Novotná V., Glogarová M.: Liquid Crystalline Benzothiophene Derivatives. *Liq. Cryst.* 35(1), 21-31 (2008).

3. Pošta M., Čermák Jan, Sýkora J., Vojtíšek P., Císařová I., Fajgar R.: Square-Planar Diphosphinoazine Rhodium(I) Amido Carbonyl Complexes with an Unsymmetrical PNP' Pincer-type Coordination. *J. Organomet. Chem.* 693(11), 1997-2003 (2008).
4. Schraml J., Cigler P.:  $^{15}\text{N}$ - $^1\text{H}$  and  $^{15}\text{N}$ - $^{13}\text{C}$  Couplings in  $^{15}\text{N}$ -Enriched Dihydroxamic Acids. *Magn. Reson. Chem.* 46(8), 748-755 (2008).
5. Stibor I., Budka J., Michlová V., Tkadlecová M., Pojarová M., Cuřínová P., Lhoták P.: Systematic Approach to New Ligands for Anion Recognition Based on Ureido-4. *New J. Chem.* 1597-1607 (2008).
6. Storch J., Čermák Jan, Pošta M., Sýkora J., Císařová I.: Palladium(II) Aryl-amido Complexes of Diphosphinoazines in Unsymmetrical PNP' Pincer-type Configuration. *J. Organomet. Chem.* 693(18), 3029-3034 (2008).
7. Sychrovský V., Benda L., Prokop A., Blechta V., Schraml J., Špirko V.: Probing the Flexibility of Internal Rotation in Silylated Phenols with the NMR Scalar Spin-Spin Coupling Constants. *J. Phys. Chem. A* 112(23), 5167-5174 (2008).
8. Sýkora J., Blechta V., Soukupová L., Schraml J.:  $^{29}\text{Si}$  -  $^{13}\text{C}$  Spin-Spin Couplings over a Si-O-Csp<sup>3</sup> Link. *Magn. Reson. Chem.* 46(12), 1112-1118 (2008).
9. Sýkora J., Karban J., Císařová I., Hilgard S.: Molecular Structure of Eight Possible Configurational Isomers of 2,3- and 3,4-Epimino Derivatives of 1,6-Anhydro- $\beta$ -D-Hexopyranoses: Conformation Analysis, Intra and Intermolecular Hydrogen Bonds. *Carbohydr. Res.* 343(16), 2789-2796 (2008).
10. Šabata S., Lehnert R., Karban J., Hetflejš J., Kuncová G.: Dekontaminace podzemní vody obsahující terc-butylmethyleter a aromatické uhlovodíky fotolýzou peroxidu vodíku. (Czech) Decontamination of Ground Water Containing tert-Butyl Methyl Ether (MTBE) and Aromatic Compounds (BTEX) by Photolysis of  $\text{H}_2\text{O}_2$ . *Chem. Listy* 102(12), 1115-1120 (2008).
11. Blechta V., Schraml J.: Measurement of Small Long-Range Couplings between Heteronuclei ( $^{29}\text{Si}$ - $^{13}\text{C}$ ) at Natural Abundance. *Magn. Reson. Chem.*, submitted.
12. Gulková D., Kaluža L., Vít Z., Horáček J., Macháčková E., Zdražil M.: High Surface Area Hydrodesulfurization  $\text{MoO}_3/\text{TiO}_2$  Catalysts. *Reac. Kinet. Catal. Lett.*, in press.
13. Pošta M., Čermák Jan, Vojtíšek P., Sýkora J., Císařová I.: Diphosphinoazine Rhodium(III) and Iridium(III) Octahedral Complexes. *Inorg. Chim. Acta*, in press.
14. Šabata S., Blechta V., Karban J., Pleska A., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-Butenes. *Phosphorus, Sulfur and Silicon*, submitted.
15. Topka P., Zub Y.L., Karban J., Šolcová O.: Designing (Al)-SBA-15 Catalyst Pellets with Unique Properties. *Stud. Surf. Sci. Catal.*, in press.

#### Chapters in books

16. Blechta V.: Applications of  $^{29}\text{Si}$ - $^{13}\text{C}$  Coupling Constants. In: *Annual Reports on NMR Spectroscopy*. (Webb, G.A., Ed.), Elsevier, Amsterdam, in press.

#### International conferences

17. Blechta V., Schraml J.: Measurement of Relative Signs of  $^{29}\text{Si}$ - $^{13}\text{C}$  Couplings. 23rd NMR Valtice, Sborník abstraktů, p. C-27, Valtice, Czech Republic, 20-23 April 2008.
18. Blechta V., Sýkora J., Kurfürst M., Schraml J.: LC- $^{29}\text{Si}$ -NMR of Organosilicon Polymers. *Magnetic Moments in Central Europe 2008*, Program and Book of Abstracts, p. 16, Ljubljana, Slovenia, 29 February 2008.
19. Gulková D., Kaluža L., Vít Z., Horáček J., Macháčková E., Zdražil M.: High Surface Area Hydrodesulfurization  $\text{MoO}_3/\text{TiO}_2$  Catalysts. 18th International Congress of

- Chemical and Process Engineering CHISA 2008, Summaries 1, pp. 97-98 (2 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
20. Chlebek J., Musilová L., Jun D., Opletal L., Kurfürst M., Schraml N., Dohnal V., Jahodář L.: Vliv isochinolinových alkaloidů z frakce A (Cl<sup>-</sup> nerozp. v CHCl<sub>3</sub>/fenolické) z *Corydalis Cava* (Fumariaceae) na cholinesterázy. (Czech) Influence of Isochinolinic A-Fraction (Phenolic CHCl<sub>3</sub> Insoluble Cl<sup>-</sup> > Salts) Alkaloids from *Corydalis Cava* (Fumariaceae) on Cholinesterases. 37. Konference Syntéza a analýza léčiv, Book of Abstracts, Chemické Listy 102 (Issue 14), s221-s222, Brno, Czech Republic, 08-10 September 2008.
  21. Kurfürst M., Schraml J.: LC-<sup>29</sup>Si NMR Analysis of Silicon Copolymer Mixtures. International Conference on LC-NMR and Related Techniques: "Challenges in Biological Systems", Program - Abstract - Information, p. 35, Jena, Germany, 27-29 August 2008.
  22. Opletal L., Cahlíková L., Dohnal V., Kurfürst M., Schraml J., Jun D., Musilová L., Doležal J., Jahodář L.: Screeningová studie vlivu některých alkaloidů z *Eschscholtzia Californica* Cham. (Papaveraceae) na lidskou erytrocytární acetylcholinesterasu. (Czech) Screening Study of Influence of Selected Alkaloids from *Eschscholtzia Californica* Cham. (Papaveraceae) on Human Erythrocytal Acetylcholinesterase. 37. Konference Syntéza a analýza léčiv, Book of Abstracts, Chemické Listy 102 (Issue 14), s238, Brno, Czech Republic, 08-10 September 2008.
  23. Sajfrtová M., Sovová H., Karban J., Pavela R.: Insecticide Activity of Herb Extracts Isolated by Different Methods. 18th International Congress of Chemical and Process Engineering CHISA 2008, Summaries 2, p. 541 (7 pp. full text on CD-ROM), Praha, Czech Republic, 24-28 August 2008.
  24. Schraml J., Blechta V., Sýkora J., Kurfürst M.: Current Topics in <sup>29</sup>Si NMR of Solutions. SMASH 2008, Conference Program, p. 1, Santa Fe, New Mexico, Mexico, 07-10 September 2008.
  25. Schraml J., Cigler P.: <sup>15</sup>N Couplings in Dihydroxamic Acids. 23rd NMR Valtice, Sborník abstraktů, p. C-28, Valtice, Czech Republic, 20-23 April 2008.
  26. Sychrovský V., Benda L., Prokop A., Blechta V., Schraml J., Špirko V.: Probing the Flexibility of Internal Rotation in Silylated Phenols with the NMR Scalar Coupling Constants. 23rd NMR Valtice, Sborník abstraktů, p. C-29, Valtice, Czech Republic, 20-23 April 2008.
  27. Sýkora J., Storch J., Karban J., Čermák Jan: Atropisomerism of 1,8-bis-(2-Propynyl-phenyl)-naphthalene. International Conference on LC-NMR and Related Techniques: "Challenges in Biological Systems", Program - Abstract - Information, p. 20, Jena, Germany, 27-29 August 2008.
  28. Šyc M., Pekárek V., Fišerová E., Karban J., Punčochář M.: The Effect of MSWI Start-up and Shut-down on Congener Profiles of PCDD/F Precursors. 28th International Symposium on Halogenated Persistent Organic Pollutants-Dioxin 2008, Organohalogen Compounds, Vol. 70, pp. 001810-001813, Birmingham, Great Britain, 17-22 August 2008.

## Miscellaneous

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### Hála Lectures

First (1999)	Arnošt REISER (Polytechnic University, Brooklyn, New York, USA) "Remembering Eduard Hála"
Second (2000)	Gerhart EIGENBERGER (Universität Stuttgart, Stuttgart, Germany) "Membrane Fuel Cell Systems: A Challenge for Chemical Engineers"

- Third (2001) David AVNIR (Hebrew University, Jerusalem, Israel)  
"The Measurement of Symmetry and Chirality: Concept and Applications across Chemistry"
- Fourth (2002) William R. SMITH (Guelph University, Guelph, Canada)  
"Macroscopic- and Microscopic-Level Thermodynamics: Partners in Chemical Engineering Progress"
- Fifth (2003) Jakob de SWAAN ARONS (Delft University of Technology, the Netherlands) "Economy, Ecology and Thermodynamics"
- Sixth (2004) Vladimír HLAVÁČEK, (State University of New York, Buffalo, USA)  
"Reactivity, Stored Energy, and Dislocations in Solid Reacting Systems"
- Seventh (2005) Jean-Claude CHARPENTIER (President of EFCE, CNRS–INPL, Nancy, France)  
"In the Frame Globalization and Sustainability: Evolution of Chemical and Process Engineering – Progression from Commodities to New Specialties and Active Material Chemistry"
- Eighth (2006) Vladimír BÁLEŠ (Slovak Technical University, Bratislava, Slovakia)  
"Trends in Research and Preparation of Technical Intelligence with Special Regard to Chemical Engineers"
- Nineth (2007) Akihiro OUCHI (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan)  
"Development of efficient multiphoton processes and their application to the studies of short-lived intermediates"
- Tenth (2008) Jan GENZER (North Carolina State University, Raleigh NC, USA)  
"“Soft material” surface engineering: from flexible to gradient surfaces"