

Academy of Sciences of the Czech Republic

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

**Praha**

ANNUAL REPORT 2007

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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)	Eva Melková
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 25)  
Department of Multiphase Reactors (page 35)  
Department of New Processes in Chemistry and Biotechnology (page 45)  
Environmental Process Engineering Laboratory (page 51)  
Laboratory of Aerosol Chemistry and Physics (page 58)  
Laboratory of Laser Chemistry (page 65)  
Department of Analytical Chemistry (page 70)

**STAFF**

(31 December 2007)

Category	Number of Employees
Research	131
Technical	20
Administrative	15
Services	15

**BUDGET 2007**

(20 Kč ≈ 1 US\$, 28 Kč ≈ 1 EUR)

Resources	Million Kč
Institutional support based on Institutional Research Plan	75
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	36
Foreign R&D Funds and European Programmes	7
Contracts with industry	4
Total Resources	122

Expenses	Per cent of Total Resources
Personal expenses including mandatory insurance	64
Purchase of material	13
Purchase of services	5
Repairs and maintenance	6
Depreciation of fixed assets	3
Travel expenses	4
Energy, water, and fuels	4
Total other expenses	1

## 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. Heyrovsky 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.

## Department of Separation Processes

Head: V. Jiříčný  
Deputy: A. Heyberger  
Research staff: J. Hanika, L. Hanková, L. Holub, P. Izák, K. Jeřábek, M. Kohoutová,  
R. Petříčkovič, M. Rousková, J. Rezníčková, M. Sajfřtová, K. Setničková,  
H. Sovová, P. Uchýtil, E. Volaufová  
Part time: V. Staněk, H. Vychodilová  
Technical staff: A. Kadlecová, D. Karfík, M. Koptová, D. Vlček  
PhD students: J. Křišťál, K. Rochová, K. Soukupová, P. Stavárek

### Fields of research

- Hydrodynamic study of dynamic behaviour of two-phase cocurrent gas-liquid pulse flow in packed bed column
- Hydrodynamics of two phase flow in narrow channel
- Liquid extraction of tall oil from wastewaters of paper industry
- 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 membrane swelling during vapour permeation and pervaporation, transport of binary mixture in polymeric membranes
- Study of vapour condensation effect in ceramic membranes pores on permeate flux
- Pervaporation and nanofiltration with ionic liquids

### Applied research

- Intensification and safety operation of trickle bed reactors under conditions of liquid phase pulse flow
- Extraction of polyaromatic hydrocarbons from aromatic petroleum fraction (300–400 °C)
- Extraction and production of plastic modifiers for production of tyres
- Refining of plant extracts
- Extraction and refining of plant extracts
- 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 study of two-phase flow in narrow channel has been conducted and two novel electrochemical reactors designed and manufactured. Another our activity consists in the implementation of numerical simulations for the prediction of two-phase flows in narrow channels. The results of this research are a part of the research in several subtasks of the project. [Refs. 17, 43-45]

### **New procedures for an operation of industrial trickle bed reactors – intensification and safety control**

(V. Jiříčný, joint project with ICT and Research Institute of Inorganic Chemistry, Ústí nad Labem, supported by MIT, TANDEM project No. FT-TA/039)

Project is focused on the research and development of the know-how [Refs. 7, 13, 22, 26, 27, 69] and method of intensification [Refs. 35, 38, 56, 70, 71] and safe control [Refs. 35, 38] of industrial trickle bed reactors. The effect of liquid feed rate modulation and hydrodynamics of liquid pulse flow on conversion and selectivity of high-pressure hydrogenation process was studied [Refs. 55, 56, 66, 67, 69]. Presentation of project results for scientific and industrial community took place at seminar in Research Institute of Inorganic Chemistry, Ústí nad Labem (December 2007). All published results and design of modification industrial size production unit for hydrogenation of pyrolysis gasoline (DPG process) were summarized on CD ROM edited for this event.

### **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. 51-53]

### **Enzymatic catalysis in supercritical carbon dioxide**

(H. Sovová, joint project with IOCB, supported by MEYS, COST project D30.001)

Enzymatic hydrolysis of blackcurrant seed oil in supercritical carbon dioxide in a continuous-flow reactor was studied with the aim to change the fatty acid composition of lipid classes in the hydrolysate by the action of stereospecific lipase Lipozyme. The reaction rate was found to depend on both Michaelis-Menten kinetics and mass transfer [Refs. 25, 65]. HPLC methods were applied to analyse the fatty acid composition of free acids [Ref. 12] and the profile of triacylglycerols [Ref. 73] in the hydrolysate. A method for estimating the stereospecific distribution of fatty acids in triacylglycerols on the basis of the data from HPLC analysis was proposed [Ref. 23]. The class of free fatty acids was found to be enriched in

saturated fatty acids and alpha-linolenic acid, while di- and monoacylglycerols were enriched in gamma-linolenic and stearidonic acids [Refs. 63, 64].

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

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

Axial mixing in a packed-bed extractor is measured using the tracer-response method; a difference between the dense CO<sub>2</sub> upflow and downflow modes is expected. The effect of material pretreatment by the instantaneous controlled pressure drop process (DIC) on the rate of oil extraction from soya beans was evaluated [Refs. 21, 50]. For the adjustment of the conditions for the fractionation of outflowing mixture of extracted substances dissolved in dense CO<sub>2</sub>, phase equilibrium of several solutes was studied, namely menthol [Ref. 11], tocopherols, beta-carotene, vitamin K<sub>1</sub> and beta-sitosterol [Ref. 61], and the class of free fatty acids as a pseudo-component in the hydrolysate of blackcurrant seed oil. The equilibrium during the extraction of minor non- and low-polar compounds was characterised by separation factors.

### **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 part of the project solved in the ICPF concerns the supercritical fluid extraction of phytosterols and phytoecdysteroids from different plants rich in these substances. Maize germ, safflower, lettuce, sea buckthorn, and *Ajuga reptans* were among the extracted plants. To dissolve phytoecdysteroids, supercritical CO<sub>2</sub> was modified with ethanol. The extraction of 20-hydroxyecdysone from the leaves and root of *Leuzea carthamoides* was studied in detail [Refs. 24, 61]. The conditions for increasing of beta-sitosterol content in oil extracted from seeds were examined [Ref. 49].

### **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 [Refs. 1, 3, 10], hydrodistillation, and Soxhlet extraction. The isolates prepared and analysed for essential oil components in the ICPF were submitted for evaluation of their insecticidal properties. Among the isolates from savory and peppermint, the highest insecticidal activity against the larvae of housefly and *Spodoptera littoralis* showed essential oils and supercritical extracts obtained at relatively mild pressure [Ref. 54]. TLC techniques for the analysis of lignans in the extracts from plants were reviewed [Ref. 28].

### **Relations between morphology and activity of polymer-supported catalysts**

(K. Jeřábek, supported by ICPF)

The project is connected with our long-time research of morphology of swollen functional polymers [Ref. 37]. In cooperation with Italian colleagues from Padua University, Italy, we studied the metal nanoparticle catalysts supported in polymer gel networks [Refs. 4-6, 15].



**Polymer adsorbents additionally crosslinked using residual double bonds – synthesis, characterization and applications**

(K. Jeřábek, supported by MEYS, project No. 1P05ME740)

We have investigated possibilities of modification of the morphology of polymer adsorbents by post-polymerization crosslinking through radical activation of residual double bonds. The morphology changes were examined by various techniques, including conventional nitrogen sorption porosimetry, inverse steric exclusion chromatography [Refs. 29, 30], scanning electron microscopy, and others.

**Study of transport phenomena in polymeric membrane during pervaporation**

(P. Uchytil, supported by ASCR, grant No. IAA4072402)

We continued the measurements on our developed sweeping-gas apparatus with a new type of a permeation cell which enables to determine amount of permeate sorbed in a membrane in a steady state of a vapor permeation process without need of any manipulation with the membrane. Data on permeate sorption in the membrane provide important information about the transport mechanism in polymeric membranes [Refs. 19, 47, 59, 60, 72]. We prepared new apparatus for measurements of the transport parameters of binary mixtures in polymeric membranes. We studied the mutual influence of binary mixtures (water - butanol) transport in linear low-density polyethylene (LLDPE) membrane. Interesting data were obtained and now the publication is prepared.

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

(P. Uchytil, joint project with ICT, JH IPC, and University of Pardubice, supported by ASCR, project No. 1QS401250509)

In collaboration with the group of Prof. Andreas Seidel-Morgenstern (Otto von Guericke University of Magdeburg, Max-Planck Institute, Magdeburg) equilibrium of gas phase adsorption on Vycor glass has been investigated. Adsorption isotherms for propane, carbon dioxide and butane as pure gases, binary mixtures and ternary mixtures were determined experimentally as a function of temperature using a volumetric method. The single component isotherms were described with the Langmuir and Freundlich equations. Additionally, a second order isotherm based on statistical thermodynamics and an isotherm equation based on vacancy solution theory taking into account real phase behavior were used for fitting single component equilibrium data. [Refs. 14, 16]

**Flow of saturated vapor through porous membranes**

(P. Uchytil, joint project with Technische Universität Wien, supported by MEYS, KONTAKT project No. 6-06-2)

In the course of the project, valuable experimental data about permeant condensation was collected. The mass flow was measured for membranes which had different pore sizes, but which were otherwise quite similar. In literature, mass flux data is rarely reported for varying pore sizes, with all the other parameters kept constant. A significant difference in the mass flux between the membranes with hydrophilic and hydrophobic surfaces was not found. Due to the small surface tension of the fluids that were used in the experiments the contact angle on differently treated membranes did not differ significantly. Some of the results were already presented in the conference [Ref. 57]. At present, the experimental results are still compared with the theoretical predictions and a manuscript that reports on the results from the collaboration is in preparation.

### **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)

The efficiency of these membrane processes is closely connected with the transport of separated substances through membranes. The development of new transport models in polymeric membranes (dense membranes) and in porous inorganic membranes (with asymmetric porous structures) based on experimental data is the main intention of our investigation.

### **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 [Ref. 8, 39] 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 [Refs. 40-42]. 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.

## **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: Separation of mixtures ethanol/toluene on cellulose myristate membrane

Institute für Mikrotechnik Mainz, Mainz, Germany: Research and development of micro devices

Otto von Guericke University of Magdeburg, Magdeburg, Germany: Influence of capillary condensation effects on 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

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

University of Colorado, Boulder, USA: Mass transport during vapour permeation and pervaporation

## Visits abroad

A. Heyberger: CSIR of Johannesburg and Durban, Republic of South Africa (4 weeks)

P. Izák: University of Lisboa, Portugal, and University of Rostock, Germany (1 month)

## 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

T. Akramov, Bashkir University, Ufa, Russia

## Teaching

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

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

J. Hanika: ICT, course "Pharmaceutical engineering"

J. Hanika: University of Pardubice, course "Industrial catalysis"

## Publications

Original papers

1. Aleksovski S.A., Sovová H.: Supercritical CO<sub>2</sub> Extraction of *Salvia officinalis* L. J. Supercrit. Fluids 40(2), 239-245 (2007).
2. Bělohav Z., Břenková L., Hanika J., Durdil P., Rapek P., Tomášek V.: Effect of Drug Active Substance Particles on Wet Granulation Process. Chem. Eng. Res. Des. 85(A7), 974-980 (2007).
3. Bocevska M., Sovová H.: Supercritical CO<sub>2</sub> Extraction of Essential Oil from Yarrow. J. Supercrit. Fluids 40(3), 360-367 (2007).
4. Bolfa C., Zoleo A., Sassi A.S., Maniero A.L., Pears D., Jeřábek K., Corain B.: Cross-Linked Poly-Vinyl Polymers versus Polyureas as Designed Supports for Catalytically Active M0 Nanoclusters. Part I. Nanometer Scale Structure of the Polyurea Support EnCat<sup>TM</sup> 40. J. Mol. Catal. A-Chem. 275(1-2), 233-239 (2007).
5. D'Archivio A.A., Tauro L., Galantini L., Panatta A., Tettamanti E., Giammatteo M., Jeřábek K., Corain B.: Cross-Linked Poly-4-vinylpyridines as Useful Supports in Metal Catalysis: Micro- and Nanometer Scale Morphology. J. Mol. Catal. A-Chem. 268(1-2), 176-184 (2007).

6. De Zan L., Gasparovičová D., Králik M., Centomo P., Carraro M., Campestrini S., Jeřábek K., Corain B.: Nanoclustered Palladium(0) Supported on a Gel-Type Poly-acrylonitrile–N,N-dimethylacrylamide–Ethylendimethacrylate Resin: Nanostructural Aspects and Catalytic Behaviour. *J. Mol. Catal. A-Chem.* 265(1-2), 1-8 (2007).
7. Hanika J., Jiříčný V., Karnetová P., Kolena J., Lederer J., Skála D., Staněk V., Tukač V.: Trickle Bed Reactor Operation under Forced Liquid Feed Rate Modulation. *Chem. Industry Chem. Eng. Q.* 13(4), 192-198 (2007).
8. Izák P., Hovorka Š., Bartovský T., Bartovská L., Crespo J.G.: Swelling of Polymeric Membranes in Room Temperature Ionic Liquids. *J. Membr. Sci.* 296(1-2), 131-138 (2007).
9. Kaštánek F., Maléterová Y., Kaštánek P., Rott J., Jiříčný V., Jiráková K.: Complex Treatment of Soils, Waste Water and Groundwater Contaminated by Halogenated Organic Compounds. *Desalination* 211(1-3), 261-271 (2007).
10. Sovová H., Opletal L., Bártlová M., Sajfrtová M., Křenková M.: Supercritical Fluid Extraction of Lignans and Cinnamic Acid from *Schizandra chinensis*. *J. Supercrit. Fluids* 42(1), 88-95 (2007).
11. Sovová H., Stateva R.P., Galushko A.A.: High-Pressure Equilibrium of Menthol + CO<sub>2</sub>. *J. Supercrit. Fluids* 41(1), 1-9 (2007).
12. Sýkora J., Bernášek P., Zarevúcka M., Kurfürst M., Sovová H., Schraml J.: High-Performance Liquid Chromatography with Nuclear Magnetic Resonance Detection — A Method for Quantification of Alpha- and Gamma-Linolenic Acids in Their Mixtures with Free Fatty Acids. *J. Chromatogr. A* 1139(1), 152-155 (2007).
13. Tukač V., Šimíčková M., Chyba V., Lederer J., Kolena J., Hanika J., Jiříčný V., Staněk V., Stavárek P.: The Behavior of Pilot Trickle-Bed Reactor under Periodic Operation. *Chem. Eng. Sci.* 62(18-20), 4891-4895 (2007).
14. Uchytíl P., Petříčkovič R., Seidel-Morgenstern A.: Transport of Butane in a Porous Vycor Glass Membrane in the Region of Condensation Pressure. *J. Membr. Sci.* 293(1-2), 15-21 (2007).
15. 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. *Chem. Eur. J.*, in press.
16. Čermáková J., Markovič A., Uchytíl P., Seidel-Morgenstern A.: Single Component and Competitive Adsorption of Propane, Butane and Carbon Dioxide on Vycor Glass. *Chem. Eng. Sci.*, in press.
17. Křišťál J., Kodým R., Bouzek K., Jiříčný V.: Electrochemical Microreactor and Gas-Evolving Reactions. *Electrochem. Commun.*, in press.
18. Kudrna V., Jahoda M., Siyakatshana N., Čermáková J., Majířová H., Machoň V.: Various Applications of the Dispersion Model for Flow Systems with Danckwerts' Boundary Conditions. *Chem. Eng. Sci.*, in press.
19. Petříčkovič R., Setničková K., Uchytíl P.: New Apparatus for Gas Permeability, Diffusivity and Solubility Assessing in Dense Polymeric Membranes. *J. Membr. Sci.*, submitted.
20. Procházka J., Heyberger A., Volaufová E.: Effect of Diluents on Sulfuric Acid Extraction with Trialkylamine. *AIChE J.*, submitted.
21. 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).
22. Skála D., Hanika J.: Dicyclopentadiene Hydrogenation in Trickle Bed Reactor under Forced Periodic Control. *Chem. Pap.*, 62(2), 215-218 (2008).
23. Sovová H., Lisa M., Holčápek M.: Estimation of Stereospecific Fatty Acid Distribution in Vegetable Oils from Liquid Chromatography Data. *Eur. J. Lipid Technol.*, submitted.
24. Sovová H., Opletal L., Sajfrtová M., Bártlová M.: Supercritical Fluid Extraction of Cynaropicrin and 20-Hydroxyecdysone from *Leuzea carthamoides*. *J. Supercrit. Fluids*, submitted.
25. 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.*, submitted.
26. Bělohav Z., Břenková L., Kalčíková J., Hanika J., Durdil P., Tomášek V., Palatová M.: Optimization of the High-Shear Wet Granulation Wetting Process Using Fuzzy Logic Modeling. *Pharm. Develop. Technol.* 12(4), 345-352 (2007).

27. Dudas J., Hanika J.: Design, Scale up and Safe Piloting of Thymol Hydrogenation and Menthol Racemisation. Chem. Eng. Res. Des., in press.

#### Chapters in books

28. Opletal L., Sovová H.: TLC of Lignans. In: Thin Layer Chromatography in Phytochemistry. (Waksmundzka-Hajnos, M. - Sherma, J. - Kowalska, T., Ed.), CRC Press, in press.

#### International conferences

29. Aleksieva K., Sassi A., Jeřábek K.: Reinforcing of Expanded Polymer Morphology Using Peroxy Radical Initiators. 34th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 141, Tatranské Matliare, Slovakia, 21-25 May 2007.
30. Aleksieva K., Sassi A., Jeřábek K.: Reinforcing of Expanded Polymer Morphology Using Peroxy Radical Initiators. European Congress of Chemical Engineering ECCE-6, Book of Abstracts, pp. 659-660, Copenhagen, Denmark, 16-20 September 2007.
31. Fialová K., Petříčková R., Uchytíl P.: Nová možnost studia "boundary layer" efektu při permeaci par. (Czech) New Possibility of Boundary Layer Effect Study during Vapor Permeation. 54. Konference chemického a procesního inženýrství CHISA 2007, Sborník 1, p. 109, Srní, Šumava, Czech Republic, 15-18 October 2007.
32. Gogová Z., Fugasová M., Hanika J.: Kinetics and Modelling of Glucose Wet Air Oxidation over Pd/C Catalyst. 34th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 309 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 21-25 May 2007.
33. Gogová Z., Fugasová M., Hanika J., Šimčík M.: Kinetics of Glucose Wet Air Oxidation using Pd/C Catalyst. EuropaCat VIII, Abstracts, P16-20 (2 pp. full text on CD-ROM), Turku/Abo, Finland, 26-31 August 2007.
34. Gogová Z., Hanika J.: Dynamický model G-L-S gas-lift s chemickou reakcí. (Slov) 54. Konference chemického a procesního inženýrství CHISA 2007, Sborník 1, p. 184, Srní, Šumava, Czech Republic, 15-18 October 2007.
35. Hanika J., Jiříčný V., Kubička D., Lederer J., Tukač V.: Zkušenost s intenzifikací reaktoru se zkrápěnou vrstvou katalyzátoru periodickou modulací rychlosti nástřiku. (Czech) Experiences from Trickle Bed Reactor Intensification by Periodic Feed Rate Modulation. 54. Konference chemického a procesního inženýrství CHISA 2007, Sborník 1, p. 106 (9 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 15-18 October 2007.
36. Hanika J., Novák L.: Procesní inženýrství - účinný nástroj pro nové technologie. (Czech) Process Engineering - Effective Tool for New Technics. 16. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2007, Sborník přednášek, pp. 1114-1117, Milovy, Czech Republic, 16-18 April 2007.
37. Hanková L., Corain B., Jeřábek K.: Swollen-State Morphology of Cross-Linked Poly-4-vinylpyridine Useful as Metal Catalyst Support. 34th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 142 (6 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 21-25 May 2007.
38. Chyba V., Tukač V., Handlová M., Hanika J., Sazanov Z., Lederer J., Kolena J., Jiříčný V., Stavárek P., Staněk V., Kubička D., Kubičková I.: Hydrogenace nenasycených uhlovodíků ve zkrápěném reaktoru při periodické modulaci nástřiku kapaliny. (Czech) Unsaturated Hydrocarbons Hydrogenation in Trickle Bed Reactor during Periodic Feed Rate Modulation. 54. Konference chemického a procesního inženýrství CHISA 2007, Sborník 1, p. 104 (5 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 15-18 October 2007.
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## E. Hála Laboratory of Thermodynamics

Head: K. Aim  
Deputy: M. Lísal  
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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)

Third virial coefficients of argon have been calculated using a recent ab initio state-of-the-art pair potential and a new ab initio three-body potential and the results were found to

compare very well with the latest experimental results. The cavity function to second order in density and the fourth virial coefficient have been derived as functions of reduced temperature for penetrable sphere model fluids. 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 describe the main characteristic features of real fluids). Newly determined experimental data on vapour-liquid equilibria in system carbon dioxide + chloropropane have been represented by Patel-Teja and PC-SAFT equations of state. Phase equilibria in systems consisting of alkanolic acids + formamide have been determined experimentally. [Refs. 6-8, 11, 23-25, 28, 44, 45]

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

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

An apparatus for the measurements of high-pressure phase equilibria has been modified for determinations in systems of molecular liquids, namely MTBE and TAME. 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. [Refs. 32, 40, 41]

### **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 also measured for system MTBE + toluene at four temperatures and atmospheric pressure. Statistic and gnostic methods were applied to fit the incomplete data of excess volumes. [Refs. 1, 17, 33, 34, 47, 51]

### **Molecular-level simulations of chemically-reacting fluids in nanoporous materials**

(M. Lisal, supported by GACR, grant No. GA203/05/0725)

Behaviour of chemically reacting fluids in both ordered and disordered nanoporous carbons has been studied by molecular simulations, thermodynamic modelling and density functional theory. Novel simulation methodologies have been developed to predict reaction equilibrium at extreme conditions. [Refs. 3, 4, 10, 12-14, 29, 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 bulk and in confinement have been developed and tested. [Refs. 9, 15, 20, 21, 48, 49, 54]

### **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 material 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 application addressed. MULTIPRO develops polymeric resins in which nanoparticles of different nature are embedded or built in, 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. 9, 31, 48, 49, 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 new original method of Monte Carlo molecular computer simulations, wherein the entire configuration is changed in one step, has been developed [18]. The method is at least by one order of magnitude faster than the so far existing single-particle methods and seems to be useful and significant especially for complex systems with non-pair interactions. Possible universality of percolation threshold in fluid systems was discovered and a new technique for identification of infinite cluster formation was proposed [26]. A new method of direct simulation of the cooling cycle has also been designed [5]. Another original result is the proposal of a novel perturbation approach with a novel type of reference system [16]. [Further Refs. 7, 8, 22, 27, 30, 42, 52, 53, 55, 56, 58, 59]

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

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

Phase equilibria in systems with reaction, e.g. esterification [2] or transesterification [39] have been experimentally investigated. Vapour–liquid equilibria in binary and ternary systems of species with selected functional groups (tert-butyl, isopropyl, carbonyl, ether, and hydroxyl) have been measured [35]. High pressure VLE data were determined in systems with CO<sub>2</sub> [44]. Algorithms for (i) reliable evaluation of temperature-independent parameters from vapour-liquid equilibria covering a temperature range [19] and (ii) robust determination of interaction parameters in equation of state from high pressure vapour-liquid equilibrium data [36] were developed. The bibliographic database of VLE data has been published within the Landolt–Börnstein Encyclopaedia series [38] (and the second volume is in press).

**EFCE WP "Fluid Separations"**

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

Activities connected with membership of M. Bendova in EFCE Working Party on "Fluid separations".

**International co-operations**

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

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

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

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

U. S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale and molecular simulations of complex systems

Universidad Rovira i Virgili, Tarragona, Spain: Molecular-based studies of chemically reacting systems in nanoporous materials

ITODYS, University of Paris VII, France: Vapour–liquid equilibrium bibliographic database; Phase equilibria in selected systems

Oak Ridge National Laboratory, Oak Ridge, TN, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems

University of Leipzig, Leipzig, Germany: Fluids at extreme conditions

Queen's University Ionic Liquids Laboratory (QUILL), Belfast, UK: Liquid-liquid phase equilibria in systems of ionic liquids

**Visits abroad**

M. Lísal: University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)

A. Malijevský: Imperial College, London, UK (5 months)

M. Malý: DICAMP, University of Trieste, Italy (1 month)

L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

**Visitors**

B. Rousseau, F. Lahmar, Université de Paris Sud, Orsay, France

J. Bonet Avalos, Universidad Rovira i Virgili, Tarragona, Spain (1 month)

P. Cosoli, DICAMP, University of Trieste, Italy (4 months)

Z. Benková, Slovenská akadémia vied, Bratislava, Slovensko (3 months)

A. Trokhymchuk, Institute of Condensed Matter Physics, Lviv, Ukraine

P. Ungerer, Institut Français du Pétrole, Rueil-Malmaison, France

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" and "Kinetic theory"
- I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"
- I. Nezbeda, M. Předota: CU, course "Introduction to computer simulations in many particle 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

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2. Bernatová S., Aim K., Wichterle I.: Vapor-Liquid and Chemical Equilibria in the Ethanol + Ethanoic Acid System at 348.15 K. *J. Chem. Eng. Data* 52(1), 20-23 (2007).
3. Brennan J.K., Rice B.M., Lísal M.: Simulating Polymorphic Phase Behavior Using Reaction Ensemble Monte Carlo. *J. Phys. Chem. C* 111(1), 365-373 (2007).
4. Bryk P., Rżysko W., Malijevský A., Sokołowski S.: Capillary Condensation in Pores with Rough Walls: A Density Functional Approach. *J. Colloid Interface Sci.* 313(1), 41-52 (2007).
5. Figueroa-Gerstenmaier S., Francova M., Kowalski M., Lísal M., Nezbeda I., Smith W.R.: Molecular-Level Computer Simulation of a Vapor-Compression Refrigeration Cycle. *Fluid Phase Equilib.* 259(2), 195-200 (2007).
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9. Lísal M., Brennan J.K.: Alignment of Lamellar Diblock Copolymer Phases under Shear: Insight from Dissipative Particle Dynamics Simulations. *Langmuir* 23(9), 4808-4818 (2007).
10. Malijevský A.: Fundamental Measure Theory in Cylindrical Geometry. *J. Chem. Phys.* 126(13), 134710-1-134710-10 (2007).
11. Malijevský A., Karlický F., Kalus R., Malijevský A.: Third Virial Coefficients of Argon from First Principles. *J. Phys. Chem. C* 111(43), 15565-15568 (2007).
12. Malijevský A., Sokołowski S.: Monte Carlo Study of Widom-Rowlinson Interface. *J. Chem. Phys.* 126(10), 106101-1-106101-2 (2007).
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15. Mamontov E., Vlček L., Wesolowski D.J., Cummings P.T., Wang W., Anovitz L.M., Rosenqvist J., Brown C.M., Garcia Sakai V.: Dynamics and Structure of Hydration Water on Rutile and Cassiterite Nanopowders Studied by Quasielastic Neutron Scattering and Molecular Dynamics Simulations. *J. Phys. Chem. C* 111(11), 4328-4341 (2007).
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## 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
- Precipitation of ammonium aluminum alum by ammonia

### 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. 16, 65-66]

### **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. 24, 42-47, 64]

### **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. 25, 26, 59-61, 63]

### **Porous catalysts and membrane supports: a relationship between mass transport and textural properties**

(V. Hejtmánek, supported by GA CR, grant No. GA203/05/0347)

The objective of this project is a modern approach to characterization of catalyst and membrane support pore structures and the investigation of a relationship between mass transport and pore structure. The pore structure characterization (reconstruction of pore space) of macroporous solids is namely accomplished by the generation of 3D image from many serial 2D cuts of actual porous media. The reconstructed pore space serves as the key information for the development of a 3D random pore network model, which allows study of a more rational prediction of mass transport phenomena in porous solids. The application of the project results in heterogeneous catalysis, separation processes, and development of new catalysts is of primary interest. [Refs. 2, 31-32, 36]

### **Organised materials for highly selective catalytic and separation processes**

(K. Jiráťová, supported by GA CR, grant No. GD203/03/H140)

Wide research group involving mostly PhD students is mainly oriented on the cooperation among them and gaining of the co-applicant's know-how in the research areas covering the topic of the proposal. Scientific aim of the project comprises synthesis of catalytic and separation structures by methods of nanotechnologies and nanoengineering. The structural and functional characterization of the prepared materials and of the process

modeling is of primary importance. The obtained results have been presented in a number of contributions in scientific journals and international symposia. [Refs. 9, 13, 42-51, 66]

### **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)

The project deals with study of syntheses and properties of catalysts of unconventional composition intended for hydrotreating. Ni phosphide phases dispersed on mesoporous SBA-15 and CMK-5 carriers are highly active in HDS of thiophene and HDN of pyridine. The studies concerning Ir sulphide and Ir promoted Mo based catalysts in different hydrotreating reactions such as HDS, HDN and hydrogenation, have been reviewed for period of the last two decades. Catalytic activity and selectivity of alumina-supported Mo sulphide promoted by small amounts of Rh, Ru, Pd and Pt was studied in HDS of benzothiophene. The maximum activity was observed for the Pd-Mo system, showing the synergetic effect close to 4 and accompanied by suppressed formation of intermediate dihydrobenzothiophene. [Refs. 10, 28, 35, 41, 68, 69]

### **Synergistic effects in hydrodesulfurization and oxidation reactions**

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

Temperature programmed techniques were used to characterize physical-chemical properties of the Mo-containing catalysts supported over Al-MCM-41, FeMoP/TiO<sub>2</sub> and NiW/alumina catalysts of various Fe/Mo and Ni/W molar ratio and the effect of mechanochemical treatment on the properties of Co-Mo catalysts. [Refs. 11, 12, 15, 27, 62]

### **Influence of chemical and phase composition of hydrotalcite based material on the catalytic activity for nitrous oxide decomposition**

(K. JirátoVá, supported by GA CR, grant No. GA106/05/0366)

Co-Mn-Al mixed oxide catalyst was modified by small amounts of metal (Pd, Pt, Ce, La, K, Na, and Li) with the aim to improve its activity for N<sub>2</sub>O decomposition. It was found that high catalytic activity in inert gas can be obtained with optimal content of K and Na, which is connected with suitable redox and acid-base properties necessary for a high rate of N<sub>2</sub>O decomposition. [Refs. 14, 30, 33, 52-57]

### **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)

The effect of small amounts of noble metals (Pt, Pd) and other metals (La, Ce, K, Li) in the calcined Co(Mg)Mn(Al) and NiMgMn hydrotalcite-like compounds on the activity and selectivity of combustion of model VOC (toluene, ethanol). 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. [Refs. 13, 48-51]

### **Unconventional supports in catalysis over sulfides**

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

The magnitude of synergism in hydrodesulfurization activity of Co-Mo catalyst strongly depended on the support. The order of synergism was CoMo/MgO > CoMo/C > CoMo/Al<sub>2</sub>O<sub>3</sub> > CoMo/TiO<sub>2</sub> > CoMo/ZrO<sub>2</sub> > CoMo/SiO<sub>2</sub>. The order of activity was CoMo/TiO<sub>2</sub> > CoMo/C >

CoMo/ZrO<sub>2</sub>>CoMo/SiO<sub>2</sub>>CoMo/Al<sub>2</sub>O<sub>3</sub>>CoMo/MgO. Deposition of Co acetylacetonate over sulphided Mo/TiO<sub>2</sub> hydrodesulphurization catalyst increased the magnitude of promotion as compared with conventional impregnation of oxide catalyst with Co(NO<sub>3</sub>)<sub>2</sub>. [Refs. 3, 4, 38]

### **Preparation of supported catalysts by slurry impregnation**

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

A new preparation method called slurry impregnation was usefully applied to deposit MoO<sub>3</sub> onto ZrO<sub>2</sub> (S<sub>BET</sub>=108 m<sup>2</sup>g<sup>-1</sup>) and ZrO(OH)<sub>2</sub> (S<sub>BET</sub>=311 m<sup>2</sup>g<sup>-1</sup>) support. MoO<sub>3</sub> gradually formed egg-shell type concentration profile up to the point, where a saturated monolayer of Mo throughout the support particles was formed. The saturated monolayer corresponded to 3.2 and 3.5 Mo nm<sup>-2</sup> for ZrO<sub>2</sub> and ZrO(OH)<sub>2</sub>, respectively. The deposited Mo efficiently hindered sintering of the texture of originally amorphous ZrO(OH)<sub>2</sub> during calcination but was not active in hydrodesulfurization. In contrast, Mo deposited over the monoclinic ZrO<sub>2</sub> was at least as twice as active as the Mo deposited over conventional gamma-Al<sub>2</sub>O<sub>3</sub> support. MoO<sub>3</sub> catalysts supported over Al<sub>2</sub>O<sub>3</sub>, alpha-AlOOH, and ZrO<sub>2</sub> were successfully promoted by slurry impregnation method using aqueous slurries of low solubility Co and Ni carbonates and hydroxycarbonates. The method of promotion studied was more efficient than conventional promotion using aqueous solutions of Co and Ni nitrates. [Refs. 4-7, 35-39, 68, 69]

### **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. 1, 17, 18, 20-23, 58]

### **Molecular basis of structure-activity relationships**

(R. Ponec, Joint project with the Ghent University)

The project is a part of long-term collaboration with the Department of Physical and Inorganic chemistry of the Ghent University. The interest in this project is primarily focused on the design of new simple theoretical models and procedures allowing us to build up the microscopic basis both for traditional structure-activity relations as well as for the design of new theoretical QSAR models. [Ref. 18, 67]

### **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  
S. van Damme, University of Ghent, Belgium  
A. Savin, University of Paris VI, France  
M. Ludwik, Central Mining Institute, Poland

## Teaching

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

## Publications

Original papers

1. Bultinck P., Ponec R., Carbó-Dorca R.: Aromaticity in Linear Polyacenes: Generalize Population Analysis and Molecular Quantum Similarity Approach. *J. Comput. Chem.* 28(1), 152-160 (2007).
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## 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

#### **Hydrodynamic interactions of bubbles and particles in flotation process**

(M. Růžička, joint project with ICT, supported by GA CR, grant No. GA104/05/2566)

The goal of this project is the investigation of the interactions between solids and bubbles in the flotation process. Our activity is focused on the underlying physical mechanisms that control the basic steps of the interactions, namely the collision dynamics of bubbles with solids of comparable size, and the hydrodynamic and surface phenomena playing roles in the agglomerate formation and its stability. The project is designed to comprise a well-balanced composition of experimental, theoretical and CFD activities. The basic experimental tool is a sophisticated and advanced visualization technique based on digital high-speed imaging. The measured data will form a basis for theoretical considerations. The modeling concepts will be tested with CFD simulations and validated with the data. The main output will be a new concept for describing the interactions between bubbles and solids. [Refs. 11, 12, 19, 20, 25, 26, 29-33, 36, 40, 54, 56-59, 62]

#### **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. 15, 26, 29-33, 36, 39, 54, 56, 57]

### **Collision dynamics of bubbles and solid particles in liquids**

(J. Havlica, supported by GA CR, grant No. GP104/05/P554)

The project is aimed at one specific and well-defined problem from three-phase hydrodynamics: interactions between a rising bubble and a moving solid particle in a liquid. The project includes three subsequent activities: (i) preparation of experimental apparatus and developing a device for production of bubbles of desired properties, (ii) experimental study of behavior of collision of a bubble and solid particle, (iii) suggestion of a theoretical model based on the results of the measurements and comparison of these results with CFD simulations. [Refs. 18, 25-28, 51, 52]

### **Bubble growth in boiling**

(J. Vejražka, supported by GA CR, grant No. GP101/05/P229)

Objective of the project is to explain processes taking place in detachment of the vapour bubble from a heated surface during boiling. The detachment is studied experimentally for both the vapour bubble and an air bubble injected through a needle. In the latter case, the needle can be rapidly moved in order to study different forces acting on the bubble. The results are compared with results of theoretical models. The main outcome will be the basis for building new models for predictions of heat transfer in nucleate boiling. [Refs. 11, 59-61]

### **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. 6, 25, 26, 29-34, 39, 40, 44, 45, 54-57, 65]

### **Reaction and transport phenomena in complex homogeneous and heterogeneous systems**

(J. Drahoš, joint project with ICT, supported by GA CR, grant No. GD104/03/H141)

The project is aimed at the preparation of PhD students for research and production activities in modern areas of chemical, pharmaceutical, biological and process industries. It includes both theoretical and experimental work of 20 students/year of ICT and ICPF in research programs directed to studies of hydrodynamics and transport processes in multiphase tower, stirred and membrane mass exchange systems, homogeneous and heterogeneous reactors and microreactors and to the studies of effects of electric field on chemical and biological systems. [Refs. 14, 15, 22, 25, 26, 29-33, 47-49, 51, 52, 58, 59, 62, 63]

### **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.

### **Study of gas holdup non-uniformity in free bubble rise aerated vessels – extension of previous analysis**

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

Local gas hold-up distribution profiles in bubble column were compared with model solutions and the flow field variation obtained from CFD modeling was demonstrated. The effect of gas distributor on the characteristic of the gas dispersion within the bubble column was tested. [Refs. 17, 50]

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

(O. Wein, supported by ICPF)

Experimental set-up for measuring voltage-step transient limiting diffusion currents has been improved (new PC driven ADDA converter, new ED hybrid interface) and equipped with a new user-friendly software EDWORK under NI LabVIEW. Theory of direction-sensitive ED probes has been expanded to the flow of microdisperse liquid displaying Apparent Wall Slip effect. [Refs. 4, 10, 64]

### **Application of the electrodiffusion sensors for the flow diagnostics in microchannels**

(J. Tihon, supported by ICPF)

The electrodiffusion technique has been improved to become applicable for the flow measurements in microchannel devices. The technique of photolithography has used to prepare very small but precisely shaped flow sensors. To gain experience with practical measurements on microfluidic scale, the electrodiffusion sensors has been tested under steady flow conditions in straight microchannels. [Refs. 2, 8, 53]

### **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. 56, 57]

**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.14, 16, 29, 30, 36, 39, 47-49, 51, 52, 55-57, 61]

**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. 12, 29-33, 39, 54]

**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

M. Shirota, Kyushu University, Japan  
A. Sato, Kyushu University, Japan  
Y. Sawae, Kyushu University, Japan  
T. Sanada, Kyushu University, Fukuoka, Japan  
M. Watanabe, Kyushu University, Fukuoka, Japan  
M. Martin, University of Salamanca, Spain  
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

## Teaching

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

M. Večeř: TU Ostrava, courses "Process engineering" and "Chemical process modeling"  
J. Havlica: UJEP, courses "Introduction to MATLAB" and "Mathematics"

## Publications

### Original papers

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3. Kristiawan M., Sobolík V., Al Haddad M., Allaf K.: Isolation of Indonesian Cananga Oil by Instantaneous Controlled Pressure Drop: Influence of Processing Parameters on Compound Yields. *J. Chem. Eng. Jpn.* 40(11), 1021-1029 (2007).
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5. Vejražka J., Marty P.: An Alternative Technique for the Interpretation of Temperature Measurements. Using Thermochromic Liquid Crystals. *Heat Transfer Eng.* 28(2), 154-162 (2007).
6. Wein O., Večeř M., Havlica J.: End Effects in Rotational Viscometry I. No-Slip Shear-Thinning Samples in the Z40 DIN Sensor. *Rheol. Acta* 46(5), 765-772 (2007).
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### Chapters in books

12. Hladil J., Růžička M.: Stromatactic Patterns Formation in Geological Sediments: Field Observations versus Experiments. In: *Particle-Laden Flow. From Geophysical to Kolmogorov Scales.* (Geurts, B.J. - Clercx, H.J.H. - Uijtewaal, W.S.J., Ed.), pp. 85-94, Springer, Dordrecht 2007.

### International conferences

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15. Bunganič R., Růžička M., Drahoš J.: Waiting Period in the Bubble Formation Process. 34th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 281, Tatranské Matliare, Slovakia, 21-25 May 2007.
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## Department of New Processes in Chemistry and Biotechnology

Head: J. Čermák  
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### 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 project was mainly focused on the optimization of the environmentally friendly reaction of reductive dehalogenation using various types of micro- and macroparticles of bimetallic catalysts as a package in reactive barriers, composed namely from Pd/Fe, Ni/Fe and Zn/Fe. The comparison of the efficiency of dehalogenation of individual bimetallic catalysts was evaluated. Dehalogenation of polychlorinated biphenyls and volatile chlorinated hydrocarbons in aqueous solutions was demonstrated both in batch and continuous laboratory scale reactors. The best results of dehalogenation follow the sequence Pd/Fe > Ni/Fe > Zn/Fe. Nanoparticles of Fe chemically produced "in situ" as an example of dynamic reactive barrier

have been applied. In contrast to the micro- and/or macroparticles of zero-valent iron, nanoparticles of Fe exhibit the capability to partially reduce even more complex molecules like PCBs, which is a new piece of knowledge. Influence of microwaves on the reductive dehalogenation was also evaluated. [Refs. 4, 5, 11, 25, 26]

### **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)

Chemistry of some well-known C-C coupling reactions was applied to new paths for synthesis of novel materials. Suzuki and Sonogashira coupling reactions together with platinum catalyzed cycloaddition were applied to the syntheses of substituted tetrahelicenes, which are potential parts for molecular electronics. New C-C coupling catalytic reactions like hydroformylation were studied with catalysis by in situ formed rhodium(I) diphosphinoazirane complexes, the active catalysts were synthesized in stoichiometric reactions and thoroughly characterized. Dendrimers with peripheral substitution by transition metal complexes were prepared and characterized. Chemistry of the  $[(C_5Me_4C_nF_{2n+1})Rh]$  fragment was further developed, new rhodium complexes for potential applications in catalytic reactions like, e.g., hydrogenation, were synthesized and their structure determined. [Refs. 1-3, 6, 8, 14, 15, 21-24, 27, 28, 32, 33, 36]

### **Combined process for methyl tert-butyl ether (MTBE) removal from water**

(G. Kuncová, joint project with ICT, supported by GA CR, grant No. GA104/05/2637)

Technical and economical evaluation of biodegradation,  $O_3/H_2O_2$  and  $H_2O_2/UV$  oxidations and conventional methods (air stripping and carbon adsorption) resulted in a combined technology of remediation of water contaminated with MTBE. In verifying experiments with a sample of real contaminated ground water, MTBE and BTEX were degraded by  $UV/H_2O_2$  photolysis at ambient temperature in a batch UV reactor. BTEX was completely mineralized while the degradation of MTBE proceeded via TBF as the only observable reaction intermediate. The high MTBE conversion (99.8 %) was achieved with the amounts of hydrogen peroxide close to the stoichiometry of the reaction. The negative effect of BTEX on the rate of MTBE degradation was reduced either by a pretreatment of the sample with activated bentonite as a selective adsorbent of these aromatic compounds or by biodegradation. Short decontamination times show promise for continuous process. [Refs. 18, 31]

### **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. [Refs. 17, 34, 35]

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

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

The research has been focused on application of new polysiloxane based polymers for immobilization of enzymes cutinase, haloalkane dehalogenase, glucose oxidase and alcohol oxidase. The immobilizates were tested as reaction catalysts and as sensitive parts of optical

sensors for monitoring of environmental pollution and biotechnological processes. [Ref. 7, 10, 19, 20, 29, 31]

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

(J. Hetflejš, joint project with IMC, SYNPO Pardubice, and University of Pardubice, 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 suitable reactive side bonds (e.g. Si-H, Si-OH bonds). Several methods have been tested for this purpose (e.g. hydrosilylation of  $\omega$ -alkenyl derivatives of pentamethylpiperidinol and some dehydrocondensation reactions) and optimized to make these reactions convenient routes to antidegradant immobilization.

### **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. Carvalho M.F.N.N., Čermák Jan, Fernandes A.C., Ferreira A.S., Galvao A.M., Matos I., Marques M.M.: Ethylene Polymerisation by Ni-Diphosphine Azine Complexes. *Polym. Int.* 56(5), 613-620 (2007).
2. Čermák Jan, Žádný J., Krupková A., Lopatová K., Vlachová A., Nguyen Thi T.H., Šauliová J., Sýkora J., Císařová I.: Tetramethyl(perfluoroalkyl)cyclopentadienyl Rhodium(III) Complexes Containing Phosphorus and Nitrogen Monodentate Donors. Crystal Structure of  $[(\eta^5\text{-C}_5\text{Me}_4\text{C}_4\text{F}_9)\text{Rh}(\text{PPri}_3)\text{Cl}_2]$ . *J. Organomet. Chem.* 692(7), 1557-1570 (2007).
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20. Bolyó J., Kuncová G.: Optické monitorovanie kyslíka a glukózy v priebehu fermentačného procesu v bioreaktore. (Slov) XVI. Medzinárodná konferencia o analytických metódach v potravinárstve, v súlade s harmonizáciou legislatívy EU Laboralim 2007, Zborník prednáškových a posterových príspevkov, p. 81-88, Banská Bystrica, Slovakia, 07-08 February 2007.



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36. Storch J., Červenková Šťastná L., Čermák Jan: Synthesis of 1-Substituted Benzo[c]phenanthrenes, Precursors for Higher Helicenes. 15th European Symposium on Organic Chemistry, Book of Abstracts, p. P328, Dublin, Ireland, 08-13 July 2007.
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## 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
- Microwave activation of heterogeneous catalytic reactions
- Effect of microwave radiation on photochemical reactions

### 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
- Microwave sintering of alumina
- Microwave depolymerization of waste poly(ethylene terephthalate) and polyurethane foams

### Research projects

**Demonstration of the production and utilization of synthetic natural gas from solid biofuels (SYNGAS)**

(M. Punčochář, supported by STREP, project No. TREN/05/FP6EN/S07.56632/019895)

The objective of the project is to realise and demonstrate the production of Synthetic Natural Gas (SNG) from solid biofuels within an innovative, large scale gasification plant which is in operation in Austria. The task of ICPF is to determine the optimal conditions for production of producer gas suitable for methanation. Several gasification experiments were carried out in order to study the influence of selected parameters on performance of allothermal steam gasification and composition of gas. Main observed parameters were gasification temperature, the steam to biomass ratio and presence of CO<sub>2</sub> in gasification medium. [Refs. 30, 31, 39]

#### **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. 9, 10, 15-18, 20, 21, 41-43, 47-49]

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

(M. Punčochář, joint project with Czech University of Agriculture, 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. 37, 38, 44]

#### **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. 4, 11, 13]

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

(V. Círka, 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. 25, 27, 28, 40, 50]

### **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. 7, 8, 27, 35]

### **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 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. 7, 8, 12, 26, 34-36, 45]

### **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. 28]

### **Microwave sintering of alumina**

(M. Hájek, J. Brustman, supported by contract ICPF – Brisk, Tábor)

Sintering of alumina samples by microwave radiation has been developed obtaining higher density compared to conventional sintering process. [Ref. 22]

### **Microwave depolymerization of waste poly(ethylene terephthalate) (PET) and polyurethane (PU) foams**

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

New method for chemical depolymerization of waste PET and PU raw material providing terephthalic acid, ethylene glycol and other products has been developed. [Refs. 23, 24]

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

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

Dust pollution in Prague was evaluated with impact on chemical composition of PM<sub>10</sub> fraction in Prague tunnels. [Ref. 51]

## 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

## Visitors

N. Ascan, Anadolu University, Eskizehir, Turkey

R. Rauch, TUW, Austria

## Publications

### Original papers

1. Hartman M., Pohořelý M., Trnka O.: Fluidization of Dried Wastewater Sludge. *Powder Technol.* 178(3), 166-172 (2007).
2. Hartman M., Pohořelý M., Trnka O.: Behaviour of Inorganic Constituents of Municipal Sewage Sludge during Fluidized-Bed Combustion. *Chem. Pap.* 61(3), 181-185 (2007).
3. Hartman M., Trnka O.: Stechiometrie spalování čistírenského kalu a bioplynu. (Czech) Combustion Stoichiometry of Sewage Sludge and Biogas. *Vodní hospodářství* 57(9), 330-332 (2007).
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6. Hartman M., Trnka O., Pohořelý M.: Oxidace organického dusíku ve stechiometrických a bilančních výpočtech spalování stabilizovaného čistírenského kalu. (Czech) Oxidation of the Organic Nitrogen in Fuel-Lean Combustion Calculations of Sewage Sludge. *Chem. Listy* 101(4), 310-314 (2007).
7. Pekárek V., Punčochář M., Bureš M., Grabic R., Fišerová E.: Effect of Sulfur Dioxide, Hydrogen Peroxide and Sulfuric Acid on the De novo Synthesis of PCDD/F and PCB in the N<sub>2</sub> + 10 % O<sub>2</sub> Atmosphere under Model Laboratory Conditions. *Chemosphere* 66(10), 1947-1954 (2007).
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10. Svoboda K., Slowinski G., Rogut J., Baxter D.: Thermodynamic Possibilities and Constraints for Pure Hydrogen Production by Iron Based Chemical Looping Process at Lower Temperatures. *Energ. Convers. Manage.* 48(12), 3063-3073 (2007).

11. Trnka O., Hartman M.: Vliv změn fyzikálních parametrů fluidních vrstev na charakteristiky tlakových fluktuací. (Czech) Influence of Changes in Physical Parameters of Fluidized Beds on Its Characteristics of Pressure Fluctuations. Chem. Listy 101(6), 515-523 (2007).
12. Bureš M., Pekárek V., Ocelka T.: Thermochemical Properties and Relative Stability of Polychlorinated Biphenyls. Environ. Toxicol. Phar., in press.
13. Hartman M., Trnka O.: Physical Characteristics of Fluidized Beds via Pressure Fluctuation Analysis. AIChE J., submitted.
14. Hartman M., Trnka O.: Monitoring the Fluidization Behavior through Time Series of Pressure Fluctuations in a Bed. AIChE J., submitted.
15. Martinec J., Šen H., Svoboda K., Martincová 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.
16. Miccio F., Kalisz S., Svoboda K., Baxter D.: Combustion of Liquid Bio-Fuels in an Internal Circulating Fluidized Bed. Chem. Eng. J., submitted.
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20. 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.
21. 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., in press.

#### Patents

22. Hájek M., Brustman J.: Způsob sintrace výrobků z aluminy. (Czech) Method of Sintration of Alumina Products. Pat. No. PV 2007-70. Applied: 07.07.26.
23. Hájek M., Sobek J., Brustman J.: Způsob chemické depolymerace odpadního polyethylentereftalátu. (Czech) Method of Depolymerization of Waste Poly(ethylene terephthalate). Pat. No. PV 2007-469. Applied: 07.07.13.
24. Kruliš Z., Horák Z., Beneš H., Hájek M.: Způsob recyklace odpadních polyurethanových pěn. (Czech) Method for Recyclation of Waste Polyurethane Foams. Pat. No. PV 2007-576. Applied: 07.08.23.
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27. Církva V., Relich S.: Study of the EDLs for Photochemical Applications. 15th European Symposium on Fluorine Chemistry, Book of Abstracts, p. 193, Prague, Czech Republic, 15-20 July 2007.

28. Hájek M., Círka V., Drahoš J., Ďurovič M., Paulusová H., Weberová L.: Microwave Drying and Disinfection of Paper Documents. 5th Asia-Pacific Drying Conference, Proceedings, pp. 954-960, Hong Kong, China, 13-15 August 2007.
29. Kalisz S., Svoboda K., Robak Z., Baxter D., Andersen L. K.: Application of FT-IR Absorption Spectroscopy to Characterize Waste and Biofuels for Pyrolysis and Gasification. 6th International Conference Fuel from Waste 2007, Proceedings, pp. 1-12, Krynica, Poland, 24-26 October 2007.
30. Kameníková P., Skoblia S., Vosecký M., Pohořelý M., Punčochář M., Koutský B.: Analyzátor pro rychlé stanovení dehtů v plynu ze zplyňování biomasy. (Czech) Analyzer for Fast Determination of Tars in Biomass Producer Gases. 59. Zjazd chemikov, ChemZi 1/3, 2007, p. 141, Tatranské Matliare, Slovakia, 02-06 September 2007.
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32. Martinec J., Schosger J.P., Baxter D., Svoboda K., Martincová J.: Developments and Practical Tests of Insulating/Cooling Capsule with Sensor for In-situ Measurements of CO Concentrations on Moving Grate in MSWI. 26th Annual International Conference on Incineration and Thermal Treatment Technologies, Book of Abstracts, pp. 1-11, Phoenix, Arizona, USA, 14-18 May 2007.
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39. Punčochář M., Hoftbauer H.: Syngas - a Way to Renewable Energy. 34th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 298, Tatranské Matliare, Slovakia, 21-25 May 2007.
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42. Svoboda K., Pohořelý M., Baxter D., Miccio F., Kalisz S.: Fluidized Bed Gasification of Impregnated Wood Containing Significant Chlorine Concentrations – Impact of Operating Parameters on Producer Gas Composition, Content of Hydrocarbons and POP. Integration Workshop Zero Emission Power Generation, Proceedings, pp. 15 (22 pp. full text on CD-ROM), Gebze, Turkey, 16-18 March 2007.
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46. Veselý V., Kulaviak L.: Chemická recyklace PET lahví. (Czech) Chemical Recycling of PET Bottles. 54. Konference chemického a procesního inženýrství CHISA 2007, Sborník 1, p. 82, Srní, Šumava, Czech Republic, 15-18 October 2007.
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49. Wieczorek K., Svoboda K., Miccio F., Baxter D., Kalisz S.: Modeling of Circulating Flow of Solids between a Fluidized Bed and a Fast Fluidized Bed/Pneumatic Transport Tube Ractor Connected by Orifices. 34th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 259 (14 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 21-25 May 2007.
50. Žabová H., Církva V., Relich S., Hájek M.: Microwave Photocatalysis of mono-Chloroacetic Acid over Nanoporous Titanium (IV) Oxide Thin Films. 2nd International Conference on Surfaces, Coatings and Nanostructured Materials, Abstracts Book, pp. 223-224, Algarve, Portugal, 09-11 July 2007.
51. Tydlitát V., Kotlík B., Karban J., Schwarz J., J. Janota: Urban Dust – Chemical Composition of PM<sub>10</sub> Fraction in Prague Tunnels. European Aerosol Conference, Program and Abstracts, p. T13A023, Salzburg, Austria, 09-14 September 2007.

## Laboratory of Aerosol Chemistry and Physics

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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. [Ref. 16]

#### 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.

### **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. [Ref. 31]

### **Contribution of secondary atmospheric PM to total PM pollution loading**

(J. Smolík, supported by Ministry of Environment, project No. VaV-SM/9/86/05)

The project is aimed at characterisation of size-resolved atmospheric particulate matter (PM) in order to estimate the contribution of secondary atmospheric PM to the total PM pollution loading at suburban area of Prague. For this purpose one year semicontinuous PM sampling is performed with subsequent gravimetric and chemical analyses. The contribution of the inorganic part will be determined using ion chromatography. [Refs. 10, 29, 30, 32]

### **Composition of size-resolved atmospheric aerosol at Prague suburban area**

(J. Smolík, supported by MEYS, COST project No. OC106)

The main task of the project is the development of humidity controlled inlets for cascade impactor and SMPS and APS systems. The inlets are used in study of hygroscopicity of size-resolved atmospheric particulate matter, sampled at suburban area of Prague. [Ref. 10]

### **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.

### **Metastable water and steam**

(V. Ždímal, supported by GA CR, grant No. GA101/05/2214)

The project aims to study the properties of water and steam in metastable state. In order to obtain missing engineering data and answer fundamental problems sophisticated experiments are carried out. A device is being developed for measurement of the surface tension of supercooled water. Studies on homogeneous nucleation from supercooled water vapor are going to be performed in an extended temperature range using a shock tube and a diffusion cloud chamber. Factors influencing the supercooling limit and the kinetics of freezing are studied. Water clusters, bulk supercooled liquid and its surface are simulated using Monte Carlo and molecular dynamics. Based on both experimental and simulation results, semi-phenomenological analytical models of metastable water and water clusters are developed, enabling engineering application. [Refs. 1-5, 21-26]

### **Application of new methods of aerosol measurement for investigation of the structure of the condensation nuclei in steam turbine**

(V. Ždímal, supported by GA CR, grant No. GA101/05/2524)

The goal of this project is to determine the real structure of the heterogeneous condensation nuclei in superheated (dry) steam. The structure of heterogeneous condensation nuclei co-determines the course of steam condensation in the turbine and thus influences its energetic efficiency and the life-time of the blades. In this project, a unique approach is used to determine the structure of heterogeneous condensation nuclei, based on modern experimental methods and measuring devices, developed for investigation of atmospheric aerosol particles. A special sampling line is being developed to connect these devices, operating at laboratory conditions, to sampling ports of the turbine at high pressure and temperature. Experiments are carried out in laboratories and subsequently in a power plant. The results are compared with measured structure of the developed liquid phase, which depends on heterogeneous condensation nuclei, and with theoretical analysis. [Refs. 2-5, 20-26, 33]

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

(J. Schwarz, Czech-Belgium bilateral exchange program in the frame of Czech-Flemish bilateral scientific cooperation)

The aim of this project is to improve knowledge concerning-hygroscopic properties of atmospheric aerosols in an urban environment by joining capacities of both laboratories. Cascade impactors with constant humidity sampling inlets (dry and wet) are going to be used to obtain size resolved samples. These samples will be analysed using ion chromatography in Prague and then for water soluble carbon in Ghent laboratory. This attitude aims to assess the influence of water soluble organic carbon on hygroscopicity of separated size fractions of urban aerosols.

### **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.

**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. 4-8, 21, 22, 26, 27]

**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.

**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 PM<sub>10</sub> 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

## Visits abroad

P. Dohányosová: Universidad Rovira i Virgili, Tarragona, Spain (9 months)

L. Džumbová: Technical University of Crete, Chania, Greece (5 months)

J. Ondráček: Technical University of Crete, Chania, Greece (5 months)

## Visitors

T. Hussein, University of Helsinki, Helsinki, Finland

## Teaching

V. Ždímal: ICT, postgraduate course: "Aerosol engineering"

## Publications

### Original papers

1. Levdansky V.V., Dragun V.L., Smolík J., Ždímal V., Moravec P.: Vliyanie poverkhnostnykh effektov pri kondenzatsii para na nanorazmernoĭ chastitse imeyushei elektricheskii zaryad. (Russ) Inzh. - Fiz. Zh. [J. Eng. Phys. Thermophys. 80(1), 57-63, 2007] 80(1), 54-59 (2007).
2. Levdansky V.V., Dragun V.L., Smolík J., Ždímal V., Moravec P.: Rol' poverkhnostnykh protsessov i razmernykh effektov v formirovanii nanochastits pri osazhdenii iz gazovoi fazy. (Russ) Vestsi Nat. Ak. Nauk Belarusi, Ser. Fyz.-Tekh. Nauk 1, 68-74 (2007).
3. Levdansky V.V., Smolík J., Moravec P.: Influence of Surface Phenomena on Free-Molecule Gas Flow in Fine Channels. Int. Commun. Heat Mass Transfer 34(7), 796-800 (2007).
4. Levdansky V.V., Smolík J., Moravec P.: Indutsirovannyi izlucheniem dreif vodoroda i ego zakhvat v metallicheskikh membranakh i chastitsakh. (Russ) Inzh. - Fiz. Zh. [J. Eng. Phys. Thermophys. 80(2), 329-338, 2007] 80(2), 112-120 (2007).
5. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Vliyanie postoronnikh gazov na fazovye perekhody v nanorozmernykh kapillyarakh. (Russ) Inzh. - Fiz. Zh. 80(4), 40-44 (2007).
6. Moravec P., Smolík J., Keskinen H., Mäkelä J., Levdansky V.V.: Vapor Phase Synthesis of Zirconia Fine Particles from Zirconium tetra-tert-Butoxide. Aerosol Air Quality Res. 7(4), 563-577 (2007).
7. Moravec P., Smolík J., Keskinen H., Mäkelä J.M., Levdansky V.V.: ZrO<sub>2</sub>/SiO<sub>2</sub> Fine Particle Synthesis by MOCVD. Chem. Vapor Depos. 13(9), 474-480 (2007).
8. Levdansky V.V., Smolík J., Moravec P.: Effect of Surface Diffusion on Transfer Processes in Heterogeneous Systems. Int. J. Heat Mass Transfer, submitted.
9. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Osobennosti fazovykh perekhodov pri formirovanii nanorozmernykh aerosolnykh chastits. (Russ) Inzh. - Fiz. Zh., submitted.

10. 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.*, submitted.
11. Smolík J., Dohányosová P., Schwarz J., Ždímal V., Lazaridis M.: Characterization of Indoor/Outdoor Aerosols in a Suburban Area of Prague. *Water, Air, Soil Pollut.*, submitted.
12. 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.*, submitted.

#### Review papers

13. Brus D., Hyvärinen A.-P., 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.*, submitted.

#### International conferences

14. Brus D., Hyvärinen A.-P., Lihavainen H., Viisanen Y., Kulmala M.: Binary Homogenous Nucleation of Sulfuric Acid and Water Mixture: Experimental Device and Setup. European Aerosol Conference, p. T13A087, Salzburg, Austria, 09-14 September 2007.
15. Brus D., Hyvärinen A.-P., Lihavainen H., Viisanen Y., Kulmala M.: Binary Homogeneous Nucleation of Sulfuric Acid and Water Mixture: Experimental Device and Setup. 17th International Conference Nucleation and Atmospheric Aerosols ICNAA 2007, Book of Abstracts, pp. 314-316, Galway, Ireland, 13-17 August 2007.
16. Džumbová L., Ždímal V., Schwarz J., Smolík J., Putaud J.P.: Aerosol Particle Penetration Efficiency through a Carbon Honeycomb Denuder. European Aerosol Conference, p. LP09, Salzburg, Austria, 09-14 September 2007.
17. Hovorka J., Ždímal V., Schwarz J., Wagner Z., Dohányosová P., Braniš M., Smolík J.: Seasonal Variation of Submicron Aerosol Number Size Distributions at Urban and Suburban Sites of Prague in 2004/2005. European Aerosol Conference, p. T13A229, Salzburg, Austria, 09-14 September 2007.
18. Hyvärinen A.-P., Brus D., Ždímal V., Smolík J., Kulmala M., Viisanen Y., Lihavainen H.: The Effect of Total Pressure on Nucleation in a Laminar Flow Diffusion Chamber: n-Pentanol + Helium. 17th International Conference Nucleation and Atmospheric Aerosols ICNAA 2007, Book of Abstracts, pp. 293-296, Galway, Ireland, 13-17 August 2007.
19. Hyvärinen A.-P., Brus D., Ždímal V., Smolík J., Kulmala M., Viisanen Y., Lihavainen H.: The Effect of Carrier Gas Pressure on Homogeneous Nucleation of n-Pentanol + Helium in a Laminar Flow Diffusion Chamber. European Aerosol Conference, p. T06A014, Salzburg, Austria, 09-14 September 2007.
20. Krejčí P., Němec T., Hrubý J., Ždímal V.: Laminar Co-Flow Tube: A Novel Tool to Study Sulfuric Acid - Water Nucleation. European Aerosol Conference, p. T13A025, Salzburg, Austria, 09-14 September 2007.
21. Levdansky V.V., Smolík J., Moravec P.: Effect of Surface Phenomena on Free-Molecule Gas Flow in Nanoscale Channels. 17th International Vacuum Congress IVC-17, Book of Abstracts, p. VSTP4-298, Stockholm, Sweden, 02-06 July 2007.
22. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Effect of Surface Phenomena on Condensational Growth of Nanoscale Aerosol Particles. 17th International Vacuum Congress IVC-17, Book of Abstracts, p. SSP4-240, Stockholm, Sweden, 02-06 July 2007.
23. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Influence of Size Effects on Condensation of Vapor on Small Charged Aerosol Particles. European Aerosol Conference, p. T06A022, Salzburg, Austria, 09-14 September 2007.
24. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Radiation-Induced Transport of Gas in Porous and Non-Porous Solid Membranes. Membrane Science and Technology Conference of

- Visegrad Countries PERMEA 2007, Book of Abstracts, p. 136, Siófok, Hungary, 02-06 September 2007.
25. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Size Effects in the Growth of Aerosol Nanoparticles and Their Coalescence. International Conference Nanomeeting 2007, Proceedings, pp. 419-422, Minsk, Belarus, 22-25 May 2007.
  26. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Radiation-Induced Transfer Phenomena in Nanoscale Systems. International Conference Fundamentals of Laser Assisted Micro- and Nanotechnologies FLAMN-07, Abstracts, p. 95, St. Petersburg, Russia, 25-28 June 2007.
  27. Moravec P., Smolík J., Keskinen H., Mäkelä J.M., Levdansky V.V.: Ni/NiO Nanoparticle Synthesis by MOCVD. European Aerosol Conference, p. T09A029, Salzburg, Austria, 09-14 September 2007.
  28. Ondráček J., Džumbová L., Glytsos T., Kopanakis I., Lazaridis M.: Characterization of Particulate Matter during Simulated Indoor Activities. European Aerosol Conference, p. T07A003, Salzburg, Austria, 09-14 September 2007.
  29. Schwarz J., Chi X., Maenhaut W., Civiš M., Hovorka J., Smolík J.: EC/OC at Two Sites in Prague. 17th International Conference Nucleation and Atmospheric Aerosols ICNAA 2007, Book of Abstracts, pp. 824-828, Galway, Ireland, 13-17 August 2007.
  30. Schwarz J., Smolík J., Hovorka J.: PM<sub>x</sub> Mass and Ionic Composition of PM in the NW Suburb of Prague in Relation to Meteorological Conditions. European Aerosol Conference, p. T13A046, Salzburg, Austria, 09-14 September 2007.
  31. Smolík J., Hruška A., Dohányosová P., Hussein T., Hemerka J.: Aerosol Dynamics in a Test Chamber: Experiment and Modelling. European Aerosol Conference, p. T07A009, Salzburg, Austria, 09-14 September 2007.
  32. Štefancová L., Schwarz J., Smolík J.: PM<sub>10</sub>, PM<sub>2.5</sub>, PM<sub>1</sub> Fractions of Particulate Matter in Prague during Year 2006. European Aerosol Conference, p. T19A027, Salzburg, Austria, 09-14 September 2007.
  33. Ždímal V., Brus D.: Homogeneous Nucleation Rate in Supersaturated Water Vapor. 17th International Conference Nucleation and Atmospheric Aerosols ICNAA 2007, Book of Abstracts, pp. 134-138, Galway, Ireland, 13-17 August 2007.



## Laboratory of Laser Chemistry

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### 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 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

#### Laser initiated chemical vapour deposition of nanosulphides

(J. Pola, supported by MEYS, project No. 1016/2006-32)

IR laser-induced co-thermolysis and UV laser-induced co-photolysis of two different progenitors to two different elements (silicon and chalcogen) allows chemical vapour formation and deposition of nanostructured silicon chalcogenides (SiSe [Ref. 1] and SiS [Ref. 9]) or nanostructured poly(carbosilthiane) films [Refs. 9, 16, 17]. Such laser-initiated chemistry represents novel approach to synthesis of inorganic compounds in the gas phase.

#### Laser fabrication of Fe and $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>/polymer nanocomposites of superior thermal stability

(J. Pola, supported by NATO collaborative project, project No. CLG980587)

Laser-assisted one-step procedure consisting in continuous-wave IR laser-induced and ethylene-sensitized co-pyrolysis of gaseous iron pentacarbonyl and organosilicon compounds (hexamethyldisiloxane) in argon was optimized for production of nano-magnetic Fe-based composites that were revealed to consist of Fe-based core and siloxane-based shell. The composites show superior thermal stability and sensing properties suggesting their use for detection of toxic carbon monoxide. [Ref. 8]

#### 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 toluene [Ref. 4] and diacetylene [Ref. 14] 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. With toluene, the diamagnetic, high surface area and Si/O-rich carbon composite is produced with ArF laser radiation, while the very rare ferromagnetic, low-surface area and Si/O-poor carbon composite is produced with KrF laser radiation. Heating of the carbon/silica/polyoxocarbosilane nanocomposite indicates a low-temperature formation of silicon carbide [Ref. 4]. These laser-induced processes have potential for fabrication of novel nanocomposite materials.

### **Laser-induced chemical liquid deposition of amorphous metal/polymer nanocomposites**

(J. Pola, supported by ICPF)

UV laser-induced photolysis of metal chelates like Cu(II) and Fe(II) acetylacetonates in alcohol solution has been studied with the aim to prepare nanoforms of metals. The ArF and KrF laser photolysis of the Cu chelate allows chemical liquid deposition of discontinuous and continuous films [Ref. 2] and yields Cu/polymer sols and nanocomposites [Ref. 5]. Similar UV photolysis of the Fe chelate results in the formation of Fe/polymer nanosol and nanocomposite [Ref. 15]. Both photolysis represent an easy and one-step processes for fabrication of amorphous metal/polymer nanocomposites, the materials incorporating very rare amorphous metal phase. KrF laser co-photolysis of Cu(II) acetylacetonate and 1-bromoeicosane was explored and revealed to yield CuBr/polymer colloidal solution and CuBr/polymer nanocomposite [Ref. 6]. This co-photolytic procedure is a new approach to polymer-stabilized nano-inorganic compounds.

### **Laser photooxidative degradation of S contaminants in fuel oils**

(J. Pola, supported by ICPF)

Degradation of 4,6-dimethyldibenzothiophene (DMDBT), persistent sulfur contaminant in fuel oils has been achieved in non-polar phase by laser-irradiating DMDBT alone and in the presence of hydrogen peroxide and molecular oxygen [Ref. 12]. The most efficient degradation in the presence of molecular oxygen is judged to be the first example of self-sensitized photo-oxygenation of thiophenes, in which DMDBT sequentially acts as  $^1\text{O}_2$  sensitizer and reactant.

### **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)

Using a new precursor tris(trimethylsilyl)germane by pyrolytic and laser assisted CVD, new Si/Ge/C materials were prepared. Laser-induced decomposition of tris(trimethylsilyl)germane resulted in brownish deposits with partially preserved Si-Ge bonds. For comparison to this deposition method, a conventional pyrolysis was performed which resulted in formation of Ge nanowires enveloped in Si/Ge/C material. Further heating under vacuum to higher temperature yielded thin wall  $\text{Si}_{1-x}\text{C}_x$  nanotubes. Lengths of nanowires and nanotubes ranged up to several micrometers.

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

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

IR and UV laser-induced deposition of  $\text{TiO}_2$  and Ti/O/Si films from two precursors [titanium tetraisopropoxide and tetrakis(trimethylsiloxy)titanium] was studied. The films, annealed at  $400^\circ\text{C}$  revealed photocatalytic activity in the UV light. Decomposition of both

precursors in the presence of ammonia resulted in formation of nitrogen-doped titania films. Laser ablation technique was used to prepare chromium-doped titania films. The doped films were analyzed using available 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, point project with JH IPC, IIC, and Institute of Physics of the ASCR, v.v.i., supported by GA CR, grant No. GA203/07/0546)

UV laser photolysis of cobalt tricarbonyl nitrosyl in the presence of acetylene generates black powder consisted of amorphous cobalt nanoparticles and 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 cobalt nanoparticles with diameter 20-30 nm, encapsulated in the amorphous carbon. The heating of the deposit to 600 °C results in crystallization of cobalt and better encapsulation. Higher temperature (900 °C) causes crystallization of the carbon shells and formation of diamond layers, covering the cobalt nanocrystals. Magnetic measurements revealed strong ferromagnetic behaviour of the cobalt nanoparticles at room temperature.

## **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. Santos, Institute of Structure of Materials, CSIC, Madrid, Spain

A. Ouchi, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

T. Majima, The Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan

## Publications

### Original papers

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## Department of Analytical Chemistry

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### 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 will enable otherwise difficult line assignments [Ref. 5], the LC-NMR part will focus on industrially important silicones where it offers entirely new possibilities [Ref. 2].

#### 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 2,3,4-trideoxy-2,3-epimino-1,6-anhydro- $\beta$ -D-*ribo/lyxo*-pyranoses were studied. Cleavage of suitable dianhydro derivatives (carbohydrate epoxides) appears to be the most promising synthetic approach. Hydroxyl group substitution in vicinal hydroxy aziridines by fluorine agents (typically DAST) was found less satisfactory. The study of the aziridine ring cleavage of 1,6-anhydro-2,3,4-trideoxy-2,3-tosylepimino-1,6-anhydro- $\beta$ -D-*lyxo*-pyranose continued and revealed that the nucleophilic cleavage reaction provided products of both *trans*-diaxial and *trans*-diequatorial cleavage.

## 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. Using these experiments model series of compounds are measured to produce the Karplus-type dependence of the vicinal  $^{29}\text{Si}-^{13}\text{C}$  couplings on dihedral angles and, subsequently, also the dependence on the nature of substituents (analogous to Altona-Haasenot equations). These dependences allow, together with other measurements (notably of Nuclear Overhauser Effects), studies of structure and conformation of silyl groups in solutions of organosilicon compounds and copolymers. The data, so far entirely missing for silicon, are of key importance for design of new compounds with required properties as needed by nanotechnology.

## 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

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5. Kurfürst M., Schraml J.: Spectral Assignments and Reference Data  $2J(^{29}\text{Si}-\text{O}-^{29}\text{Si})$  Coupling Constants in Oligosiloxanes. *Magn. Reson. Chem.* 45(8), 685-687 (2007).

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9. Sýkora J., Himl M., Stibor I., Císařová I., Lhoták P.: Unique Self-Assembly Patterns Based on the Thiocalix[4]arene-Silver Interactions. *Tetrahedron* 63(10), 2244-2248 (2007).
10. Blechta V., Schraml J.: Relative Signs of  $^{29}\text{Si}$ - $^{13}\text{C}$  Couplings. *Magn. Reson. Chem.*, submitted.
11. Pošta M., Čermák Jan, Sýkora J., Vojtíšek P., Císařová I., Fajgar R.: Square-planar Diphosphinoazine Rhodium(I) Amido Carbonyl Complexes with an Unsymmetrical PNP<sup>3</sup> Pincer-type Coordination. *J. Organomet. Chem.*, submitted.
12. Pošta M., Čermák Jan, Vojtíšek P., Sýkora J., Císařová I.: Diphosphinoazine Rhodium(III) and Iridium(III) Octahedral Complexes. *Inorg. Chim. Acta*, submitted.
13. 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.

## International conferences

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15. Blechta V., Sýkora J., Kurfürst M., Schraml J.: LC-NMR of Polysiloxanes. 22nd NMR Valtice, Sborník abstraktů, p. C-12, Valtice, Czech Republic, 15-18 April 2007.
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19. Krupková A., Vlachová A., Císařová I., Sýkora J., Čermák Jan: Synthesis and NMR Study of Conformational Dynamics of  $[(\text{C}_5\text{Me}_4\text{C}_n\text{F}_{2n+1})\text{Rh}(\text{LCl}_2)]$  Complexes with Nitrogen Ligands. 15th European Symposium on Fluorine Chemistry, Book of Abstracts, p. 303, Praha, Czech Republic, 15-20 July 2007.
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21. Pošta M., Čermák Jan, Vojtíšek P., Sýkora J., Císařová I.: Octahedral Rh(III) Diphosphinoazine Complexes: Synthesis and Hemilability. XVII EuCheMS Conference on Organometallic Chemistry, Book of Abstracts, p. 80, Sofia, Bulgaria, 01-06 September 2007.
22. Pošta M., Sýkora J., Císařová I., Vojtíšek P., Čermák Jan: Coordination Behaviour of Diphosphinoazine Ligands in Rhodium and Iridium Complexes. 6th International School of Organometallic Chemistry, Book of Abstracts, p. 115, Camerino, Italy, 08-12 September 2007.
23. Sajfirtová M., Sovová H., Pavela R., Karban J.: Insecticidal Activity of Herb Essential Oils Isolated Using Supercritical Fluid Extraction. 5th International Symposium on High Pressure Process Technology and Chemical Engineering, Program and Abstracts, p. 187 (9 pp. full text on CD-ROM), Segovia, Spain, 24-27 June 2007.



24. Schraml J., Blechta V., Sýkora J., Kurfürst M.: LC-NMR Analysis of Organosilicon Polymers. 4th European Silicon Days, Programme, Abstracts, and List of Participants, p. 61, Bath, Great Britain, 09-11 September 2007.
25. Schraml J., Blechta V., Sýkora J., Kurfürst M.: LC-NMR of Silicon Polymers. 5th International Workshop of Silicon-Based Polymers, Book of Abstracts, p. 35, Montpellier, France, 25-27 June 2007.
26. Sýkora J., Sovová H., Kurfürst M., Schraml J.: LC-NMR Method for Analysis of Free Fatty Acids in Natural Oils. 22nd NMR Valtice, Sborník abstraktů, p. C-11, Valtice, Czech Republic, 15-18 April 2007.

## Miscellaneous

### International Advisory Board of ICPF

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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)

- Fourth (2002) "The Measurement of Symmetry and Chirality: Concept and Applications across Chemistry"  
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"