

## Department of Catalysis and Reaction Engineering

### HEAD

**OLGA ŠOLCOVÁ**

### DEPUTY

**PETR KLUSOŇ**

### SCIENTISTS

**JANA GAÁLOVÁ, VLADIMÍR HEJTMÁNEK, LUDĚK KALUŽA, MAGDALENA MOROZOVÁ, KAREL SOUKUP, PAVEL TOPKA, ZDENĚK VÍT**

Part time: **DANIELA GULKOVÁ, KAREL JEŘÁBEK, KVĚTUŠE JIRÁTOVÁ, FRANTIŠEK KAŠTÁNEK, LENKA MATĚJOVÁ, ROBERT PONEC, MIROSLAV ZDRAŽIL**

### RESEARCH ASSISTANTS

**LADISLAV HOLUB, YWETTA MALÉTEROVÁ, MARTINA MATĚJKOVÁ, BARBORA PAPEŽOVÁ, HANA ŠNAJDAUFOVÁ**

Part time: **JANA BALABÁNOVÁ, LIBUŠE HANKOVÁ, JAN KLEMPA**

### PHD STUDENTS

**ONDŘEJ BENEŠ, PAVLÍNA DRAGONOVÁ, PAVEL DYTRYCH, PAVEL KRYSŤYNÍK, JANA LUDVÍKOVÁ, JANA PAVLORKOVÁ, LUCIE SPÁČILOVÁ**

### LAB TECHNICIANS

Part time: **JANA BUDOVIČOVÁ, HELENA SOUČKOVÁ**

## Fields of research

- Advanced catalytic oxidation processes
- Catalytic combustion of volatile organic compounds in waste gases
- Catalytic decomposition of N<sub>2</sub>O
- Design of new theoretical models for structure-activity relationships
- Morphology and application properties of catalysts based on functional polymers
- Preparation of hierarchic nanomaterials
- Temperature programmed techniques in characterization of catalysts
- Texture and transport processes in porous solids
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Preparation and characterization of the electrospun nanofibrous membranes and catalytic supports
- Unconventional preparation of metal oxide nanostructures by pressurized fluid extraction and supercritical drying

## Applied research

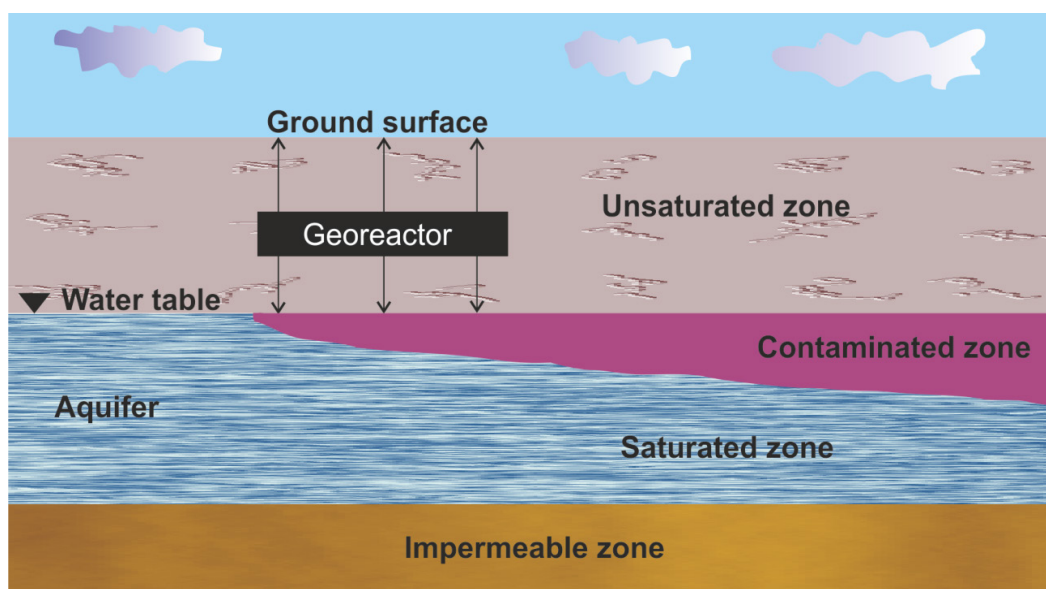
- Catalytic combustion of volatile organic compounds
- Oxidation processes for environment
- Textural characteristics of structural materials
- Green chemistry for biomass utilization to the high added-value products

## Research projects

### Hydrogen oriented underground coal gasification (UCG) for Europe - environmental and safety aspects (HUGE2)

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with GIG, Politechnika Slaska, Kompania Węglowa S.A. and Lubelski Węgiel Bogdanka S.A., Poland, Institut National de l'environnement industriel et de risques, France and UCG Engineering Ltd, UK; supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2011-00002)

This project is focused on safety and environmental aspects of underground coal gasification. Underground trial has been performed in mine testing two borehole system and reactive barriers usage. The most serious environmental concerns related to UCG have been investigated that is contamination of underground aquifers and potential leakage of poisonous and explosive gases into the surrounding strata. The work is focused on finding practical solutions of possible leakages prevention by use of reactive barriers. Complex system of environmental telemetric monitoring was built and tested. Also technical and ecological risk assessment was performed.



**Conceptual model of the contaminants migration from georeactor zone**

HUGE2 project has played a complex role in the development of the UCG technologies, an important element of Clean Coal Technology proposals for Europe. It has enabled the enhancement of the consolidation between the European laboratories involved in the development of the UCG technology as well as comprised the continuation of collaboration established within the HUGE (2007-2010) project between the European experts and the European coal companies. Necessary attention has been paid to the implementation of the UCG technologies in industry through the involvement of companies, in particular from outside of Europe. The project has helped to overcome the legal and formal restrictions through enhancing the knowledge of the environmental constrains and hazards as well as providing the tools to help overcome these constrains. It has delivered the resources and opportunities for the development of the Clean Coal Technology Centre in the Central Mining Institute. It has enabled launching PhD courses within the Polish project – Development of human resources for Clean Coal Technologies' research. The HUGE2 project has become the vehicle for other European projects dedicated to Underground Coal Gasification such as: Technology Options for Coupled Underground Coal Gasification and CO<sub>2</sub> Capture and

Storage (TOPS), Enhanced Coal Exploitation through UCG Implementation in European Lignite Mines (Coal2Gas) and Methane Production through Underground Coal Gasification from Deep European Coal Seams (MEGA). [Ref. 15]

### **Removal of heavy metals and radionuclides from water using ceramic membranes**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Institute for Single Crystals of NAS of Ukraine and University of Maribor, Slovenia; supported by NATO, project No. SFP 984398)

The problem of environmental pollution with radionuclides is especially acute in Ukraine after the Chernobyl catastrophe in 1986 which caused serious radioactive contamination of the surface aquatic environment. Even currently uranium concentration in liquid low-level radioactive wastes from the object "Shelter" in Chernobyl Exclusion Zone exceeds 30-40 mg/l. These wastes require treatment to meet discharge regulations to the inland waterways and to minimize the volume of radioactive material to be stored. Additionally, Ukraine ranks sixth place in the world and first in Europe regarding the reserves of uranium ores. Large volumes of drainage and process water contaminated with uranium and other radionuclides are formed during mining and enriching of uranium ores. Unfortunately, this polluted water as a rule enters the environment without adequate treatment.

Therefore, the main objective of the project is to develop a family of advanced nano- and ultrafiltration ceramic composite membranes containing functionalized mesoporous silica layers which will be capable of selective binding of heavy metals (Hg, Cd, Cr) and uranium from surface and waste waters and thus preventing or minimizing the environmental exposure to hazardous substances. [Ref. 19]

### **Structured catalysts with active oxide layer for removal of gaseous pollutants**

(K. Jiráťová, [jiratova@icpf.cas.cz](mailto:jiratova@icpf.cas.cz); joint project with TU of Ostrava, and UCT, Prague; supported by GACR, project No. 14-13750S)

Mechanochemical method was proposed and applied for preparation of Al-Ce mixed oxide supports of catalysts for the total oxidation of volatile organic compounds. The calcination products do not contain harmful sodium and show high surface area, large pore volume, and big average diameter of mesopores (around 8 nm). Analogous mechanochemical method was used for preparation of precursors giving the Co-Mn-Al mixed oxide catalysts after heating. The catalysts were modified with Cs promoter and showed high activity and selectivity in ammonia oxidation to  $N_2O$  at low temperatures of about 250 °C.

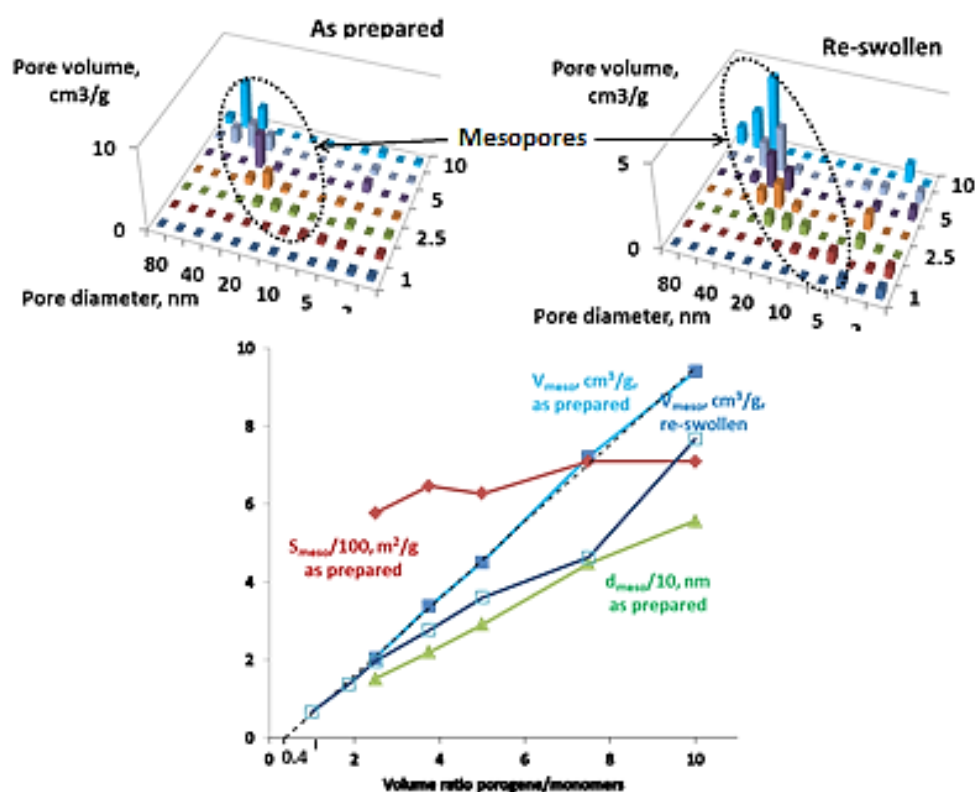
The Co-Mn-Al mixed oxide catalysts on preformed supports (alumina spheres and cordierite monoliths wash coated with alumina) were prepared and tested in the total oxidation of ethanol and decomposition of  $N_2O$ . The catalysts prepared by deposition of dried LDH precursor over alumina spheres showed the highest activity. The activity of monolithic catalysts was comparable to that of the impregnated pellets. The Co-Mn-Al mixed oxides were deposited on the supports by hydrothermal crystallization of LDH precursors and subsequent heating. The aluminum sieve and monolith with (Co+Mn) active metals exhibited comparable activity in ethanol oxidation as reference Envicat catalyst.

### **Morphology and application properties of mesoporous poly(divinylbenzenes)**

(K. Jeřábek, [kjer@icpf.cas.cz](mailto:kjer@icpf.cas.cz); joint project with Zhejiang University, Hangzhou, China; supported by MEYS, project No. LH12194)

Chinese colleagues discovered a novel polymerization method producing porous polymers with very high surface area and unique mesoporous morphology, completely different from conventionally prepared materials of similar chemical nature. In their preparation is used exceptionally high dilution of monomers with porogenic solvents. With help of inverse steric exclusion chromatography method developed in Prague providing

information on the polymer morphology in its native, swollen state undeformed are investigated relations between preparation conditions of mesoporous functional polymers and their morphology. It was found that the pore volume in the polymer examined just after preparation corresponded to the volume of the porogen used [Ref. 18]. Drying of the polymers of course induces extensive collapse of the porous structure. Water, as additive to the porogenic solvent, influences ability of the polymer morphology to re-swollen to its original state. There was found that the mesoporous morphology is formed by microsineresis rather than the macrosineresis mechanism that is common in the synthesis of conventional porous polymer materials. There were defined conditions needed for the microsineretic pore formation in highly crosslinked polymer materials allowing production of a new class of functional polymers. [Refs. 5, 6, 14, 18]



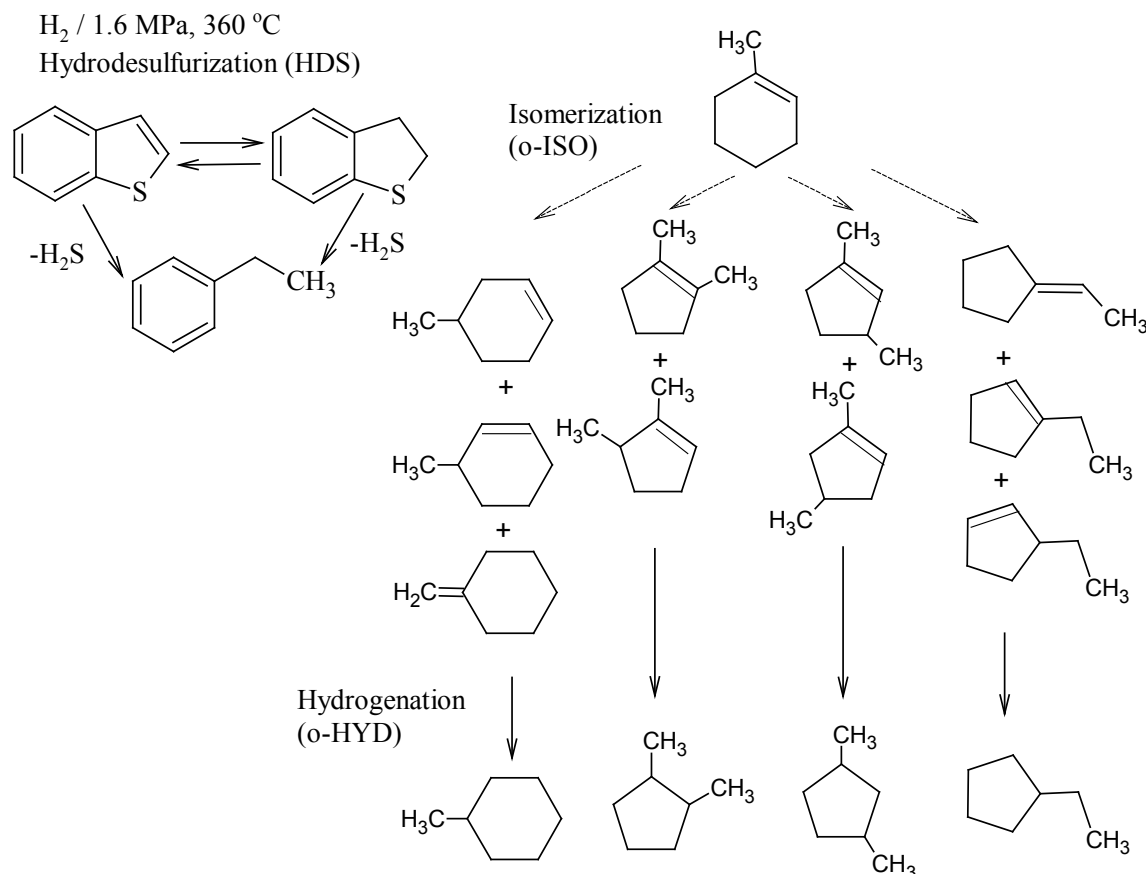
**Effect of monomer dilution (tech. DVB, 80 %) with toluene on the swollen-state morphology assessed by ISEC**

### **Unconventional composition and preparation of sulfide hydrotreating catalysts**

(L. Kaluža, [kaluza@icpf.cas.cz](mailto:kaluza@icpf.cas.cz); supported by GACR, project No. 106/11/0902)

Sulfide CoMo/Al<sub>2</sub>O<sub>3</sub> catalysts were compared with unconventional PdMo/Al<sub>2</sub>O<sub>3</sub> in hydrodesulfurization (HDS) reaction of model compounds emphasizing on the catalysts nitrogen tolerance. Furthermore, the studies were focused on elucidation of the effect of catalyst precursor and its pretreatment on the amount of β-Pd hydride phase and HDS activity over bimetallic Pd-Pt/silica-alumina. Over selected catalysts, moreover, the rearrangement of 1-methylcyclohex-1-ene during the HDS of model fluid catalytic cracking (FCC) gasoline was described. An isolation and identification of branched cyclic C7 olefins were addressed. Dimethyl-cyclopentenes and ethylcyclopentenes were determined during the simultaneous HDS of 1-benzothiophene and hydrogenation (o-HYD) of 1-methylcyclohex-1-ene. They were isolated by combination of chromatographic techniques and were undoubtedly assigned

via NMR spectroscopy. The collected  $^1\text{H}$  NMR data of individual dimethyl-cyclopentenes and ethylcyclopentenes ensures more accurate NMR prediction of cyclopentene derivatives and other related compounds in the future. The identification of the minor volatile content was found to be the crucial step in forthcoming kinetic study of the hydrogenation process. [Refs. 22, 23, 24]



### Model hydrotreating reactions for unconventional catalysts

#### Microalgae as a promising source of omega-3 unsaturated fatty acids and their incorporation into the human food chain

(F. Kaštánek, [kastanek@icpf.cas.cz](mailto:kastanek@icpf.cas.cz); joint project with Rabbit Trhový Štěpánov a.s., IBOT, EcoFuel Laboratories, Institute of Microbiology CAS, Mydlářka a.s., Rabbit CZ a.s., Rabbit Chotýšany a.s., CU, ICPF, UCT Prague; supported by TACR, project No. TA03011027)

The project is focused on utilization of the lipid new sources with the high content of the healthy polyunsaturated fatty acids (PUFAs), omega-3 types. Microorganisms, mainly biotechnologically produced eustigmatofit microalgae with the high content of PUFA, have been applied. New types of mixotrophic bioreactors were designed to obtain the optimal content PUFA in biomass. Products will be used as the feeding additives for poultry.





**The newly designed mixotrophy reactor**

### **Innovative autoMotive MEA Development - implementation of Iphe-genie Achievements Targeted at Excellence (IMMEDIATE)**

(L. Kaluža, [kaluza@icpf.cas.cz](mailto:kaluza@icpf.cas.cz); supported by European Union's 7<sup>th</sup> Framework Programme FP7/2007-2013 for the Fuel Cells and Hydrogen Joint Undertaking Technology Initiative, project No. 303466 and co-supported by MEYS, project No. 7HX13003)

Catalysts consisting of 60 wt.% of Pt were prepared by one-step impregnation of the studied high-surface-area carbon black ENSACO® 350G using  $\text{PtO}_2$ ,  $\text{H}_2\text{PtCl}_6$ ,  $\text{Pt}(\text{C}_5\text{H}_7\text{O}_2)_2$ ,  $\text{Pt}(\text{NH}_3)_4(\text{NO}_3)_2$ , and  $\text{Pt}(\text{NH}_3)_2(\text{NO}_2)_2$  solutions or slurries. These deposited species were reduced to metallic Pt at 0, 70, 120, 140, and 150 °C, respectively. Calcination in Ar followed by reduction in an  $\text{H}_2/\text{Ar}$  mixture at 190 °C ranked these catalysts in the following order of increasing Pt particle size:  $3 < 8 < 11-17 \sim 16 < 18-35$  nm for the precursor  $\text{H}_2\text{PtCl}_6$ ,  $\text{Pt}(\text{NH}_3)_2(\text{NO}_2)_2$ ,  $\text{Pt}(\text{C}_5\text{H}_7\text{O}_2)_2$ ,  $\text{Pt}(\text{NH}_3)_4(\text{NO}_3)_2$ ,  $\text{PtO}_2$ , respectively, favoring  $\text{H}_2\text{PtCl}_6$ . A dechlorination procedure based on one extraction with NaOH solution followed by intensive rinsing with distilled water was developed to decrease the level of hydrolyzable chloride well below 100 ppm in the  $\text{H}_2\text{PtCl}_6$  based catalyst. The dechlorination increased the Pt particle size from 3 to 4.5 nm.

An experimental carbon black ExpCB of intermediate surface area  $384 \text{ m}^2\text{g}^{-1}$  was compared with the 350G of  $808 \text{ m}^2\text{g}^{-1}$  and with the low surface area carbon blacks 290G and XC72 of  $226 \text{ m}^2\text{g}^{-1}$  and  $236 \text{ m}^2\text{g}^{-1}$ , respectively. Laser Raman spectroscopy revealed that all supports contained turbostratic graphitic crystallites of similar size of about 5 nm. Deposition

of 60 wt. % Pt on ExpCB by impregnation with  $\text{H}_2\text{PtCl}_6$  resulted in Pt particle sizes of 4.7 and 8.3 nm for non-dechlorinated and dechlorinated catalyst, respectively. XRD analysis practically confirmed the Pt particle size found by hydrogen pulse chemisorption in the dechlorinated  $\text{H}_2\text{PtCl}_6/\text{ExpCB}(\text{CRNaWR})$  catalyst, rendering the value of 10 nm.

Electrochemical RDE analysis indicated that impregnation by  $\text{H}_2\text{PtCl}_6$  is the most suitable of the catalyst synthesis methods applied in this study. Mass-specific ORR activities in the same order as that for the commercial reference catalyst are obtained for catalysts prepared this way. Due to better electrochemical stability the carbon ExpCB was found to be a better suited catalyst support material than 350G. The electrochemical measurements also indicated that further increase in stability is achieved by dechlorinating the catalyst according to the procedure developed in this study.

### Research and development of special dyes using ionic liquids as efficient functional additives

(P. Klusoň, [kluson@icpf.cas.cz](mailto:kluson@icpf.cas.cz); joint project with Teluria, Techem; supported by MIT, project No. FR-TI3/057)

This project deals with utilization of special types of ionic liquids based on tetra-alkyl ammonium bistriflateamides as additives for new types of dyes. These additives may bring special properties to the final product, such as higher mechanical stability, higher effect of the pigment addition and lower amounts of various pigments, more complex compositional solutions, etc. The project comprises preparation of the selected ionic liquids, their characterization by many types of physical methods (viscosity, contact angle, density, etc.), and then their direct application together with other characteristic components. The project addresses completely new way to obtain modern dyes useful both in industry as well as for standard and common customers.



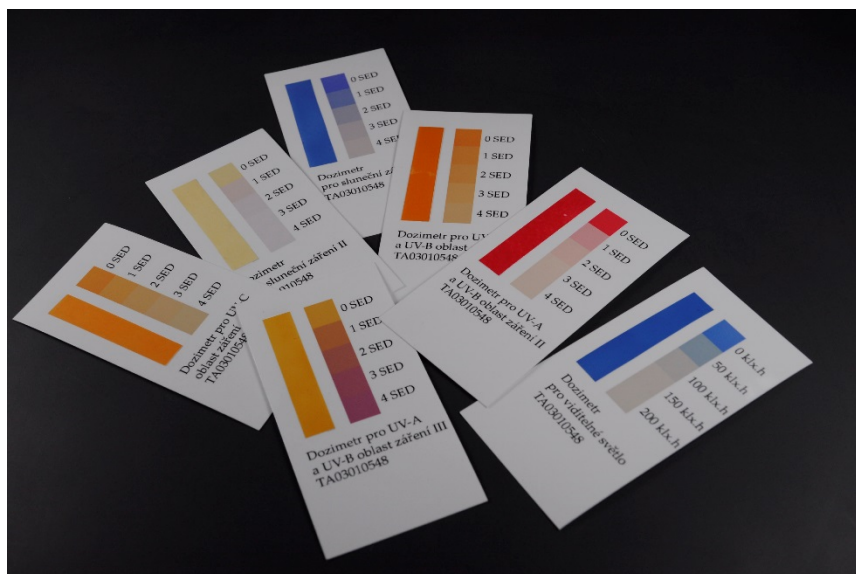
Emulsification progress with and without special additives

### Research and development of advanced thin film elements for direct evaluation of the time variable with by means of the precisely calibrated color change

(P. Klusoň, [kluson@icpf.cas.cz](mailto:kluson@icpf.cas.cz); joint project with INVOS Ltd., COC Ltd., CU, ICPF, TU Brno; supported by TACR, project No. TA03010548)

Aim of the project, shortly named *Color Clocks*, focuses on the applied research & development and testing of the advanced thin film elements for direct evaluation of the time variable by means of precisely calibrated color change. These elements represent a highly specific form for time measurement under highly specific conditions and for very specific

practical purposes. These structures are supposed to be used as tools for simple visual and intuitive evaluation of the time variable under very different circumstances. It is a kind of standard memory element collecting a certain type of data, which are then assessed in the cumulative form as the absorbed light dose of characteristic energy, or characteristic energetic region. The light sensitive films are based on uniformly organized nanoparticles that exhibit an adjustable photocatalytic activity toward the decomposition of selected organic structures deposited onto their surfaces. The decolorization process is then carefully calibrated for many different types of probe organic molecules. There are many possible practical applications of these materials, among others dermatology, conservation and storage of historical monuments and artefacts, should be mentioned. [Refs. 3, 4, 8]



UV-light exposure sensors

### Use of PFG NMR, stochastic reconstruction and molecular simulation to estimate transport-related texture characteristics of advanced porous materials

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with CU and JH IPC; supported by GACR, project No. P204/11/1206)

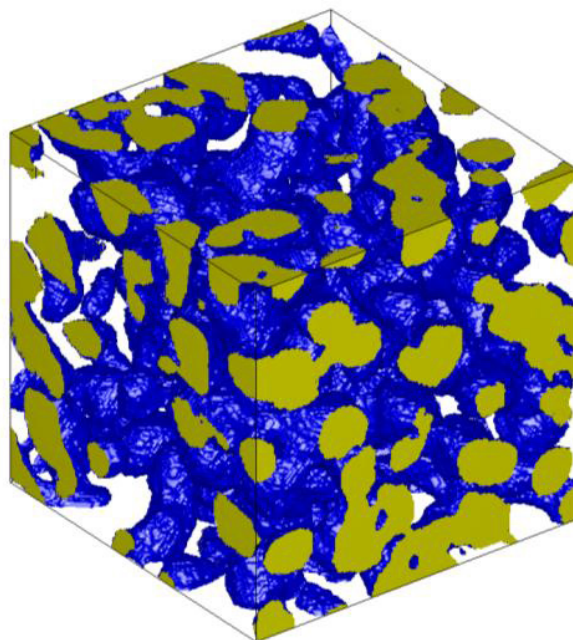
Microstructures of three mixed-matrix membrane samples made of polyimide and silicalite-1 particles were reconstructed using a stochastic reconstruction procedure. The results of this reconstruction were tested by simulating the random walk of CO<sub>2</sub> molecules in the reconstructed bodies and by predicting the effective permeability of CO<sub>2</sub>. Both original and reconstructed membranes revealed a similar enhanced effective permeability, which exceeded predictions based on the effective medium approximations. Therefore, it was suggested that clustering of the silicalite-1 particles was the primary cause of the permeability increase.

The sensitivity analysis of gas transport problems related to experimental setups that are routinely used for determination of effective transport parameters of macroporous solids is presented. The relevance of large total pressure variations to reliable estimation of the effective transport parameters is emphasized in two experimental setups, particularly quasistationary permeation and classical Wicke–Kallenbach cells.

The effective transport properties of advanced porous materials based on hydroxyapatite nanopowders were characterized by means of the effective diffusion coefficients. Polystyrene molecules substituted a role of biofluids transported in human body (especially in bones) were used as appropriate model compounds. The effective diffusion coefficients for two



polystyrene samples with different relative molecular weights (1000 and 100,000) in cyclohexane on hydroxyapatite were evaluated. It was found that the binary effective diffusion coefficients revealed much lower values in comparison with the binary bulk ones due to the strong influence of hindered diffusion in hydroxyapatite pore network. [Refs.1, 2, 16, 17]



**3D replica of mixed matrix membrane M5. The cube size is limited to 200×200×200 voxels for a clear view. The phase interface is blue. Intersections of silicalite particles and cube walls are yellow. The polyimide phase is transparent**

### **Removal of endocrine disruptors from waste and drinking water by photocatalytic and biological processes**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Dekonta, a.s. and Institute of Microbiology CAS; supported by TACR, project No. TA01020804)

Endocrine disruptors represent the group of chemical substances disrupting the hormonal indication of vertebrates and thereby they could encroach on the organism function. To the group of endocrine disruptors belong surfactants, softeners, fungicides, insecticides and some kinds of medications and hormonal contraception. They are commonly presented not only in the waste water but also in the natural water. Endocrine disruptors are persistent to degradation by common chemicals as well as biological and photolytic processes. The necessity of finding the alternative solutions leads to development and use of the new technologies. Photo-catalysis using semiconductor particles have found increasing interest to solve the endocrine disruptors remove problems.

This project is focused on verification of the specially designed photoactive materials and their modified versions suitable for photo-processes carried out upon illumination in the UV-light. Ethynylestradiol, nonylphenol and bisphenol A were chosen as typical compounds belong to the endocrine disruptor group. In this work the water decontamination with various concentrations of endocrine disruptors in the two types of reactors; batch and plug flow arrangement on the titania thin layers were successfully studied. Moreover, the application of the specially designed pilot plan photoreactor was verified on real waste water. [Refs. 9, 10, 25, 27]

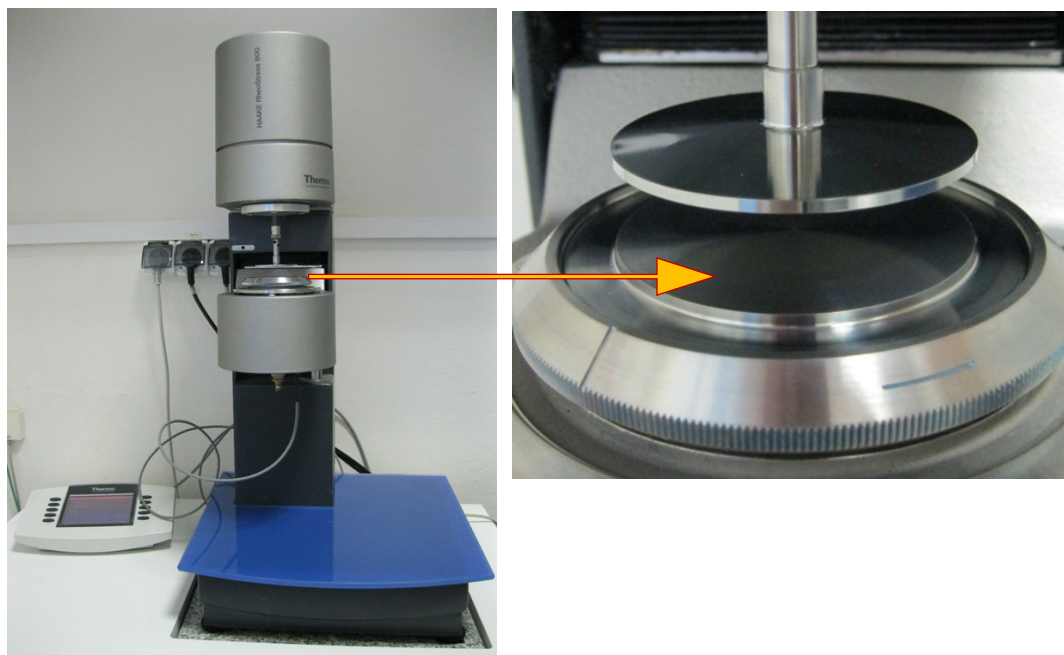


**Operational tests on sewage plant**

### **Ionic liquids as additives for special pigments**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Synthesia, a.s., TECHEM CZ, s.r.o.; supported by MIT, project No. FR-TI4/189)

Ionic liquids are composed of large ions with a low degree of the overall molecular symmetry. Very high coulombic interactions are behind their impressive electrical and mechanical stabilities, thermal and pressure resistivity, and extremely low tension of vapors. Low flammability, very good electrical conductivity, high thermal capacity and unusual phase behavior might be added to the previous list of exceptional properties. No doubts these features qualify them for a broad band applications ranging from “green solvents” due to their negligible volatility, over templates for synthesis of nanoparticles (some of them tend to form organized ionic clusters), liquid electrolytes in solar cells and fuel cells, to liquid adhesives, special lubricants, chromatography mobile phases, incombustion additives, etc. One of the most prominent applications is their use as special additives for pigments and dye compositions. If the side-chains are too short, they do not disturb the ionic network significantly and, also, they do not possess enough conformational freedom to adopt a low energy configuration. However, increasing the chain-length the role of its spatial arrangement becomes much more important. In this respect this project pays special attention to the utilization of quaternary ammonium ionic liquids, namely n-alkyl-triethyl ammonium bis(trifluoromethane sulfonyl) imides ( $N_{R222}Tf_2N$ ,  $R = 6, 7, 8, 10, 12, 14$ ) with a variable length of an alkyl chain are specially promising.



**Applied rheometer Haake RS 600 a detail of sensor panel**

### **New heterogeneous catalysts for environmental protection**

(L. Kaluža, [kaluza@icpf.cas.cz](mailto:kaluza@icpf.cas.cz); joint bilateral co-operation with Institute of Catalysis, BAS, Sofia, Bulgaria; supported by CAS)

High surface area TiO<sub>2</sub> nanotubes (Ti-NT) synthesized by alkali hydrothermal method were used as a support for NiW hydrodesulphurization catalyst. Nickel salt of 12-tungstophosphoric acid (Ni<sub>3/2</sub>PW<sub>12</sub>O<sub>40</sub>) was applied as oxide precursor of the active components. A polytungstate phase evidenced by Raman spectroscopy was observed indicating the destruction of the initial heteropolyanion. The catalytic experiments revealed two times higher thiophene conversion on NiW catalyst supported on Ti-NT than those of catalysts supported on alumina and titania. Increased HDS activity of the NiW catalyst supported on Ti-NT could be related to a higher amount of W oxysulfide entities interacting with Ni sulfide particles as consequence of the electronic effects of the Ti-NT observed with XPS analysis.

### **Enhancement of the power transformer operation security and prevention of their failures caused by the corrosive sulphur effect**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Orgrez, a.s.; supported by TACR, project No. TA04020151)

Recently, a significant volume of research has been undertaken in order to understand the failure of relatively new oil-filled transformers. The cause of failure has been a short circuit in the dielectric isolation. This effect is attributed to the so-called “corrosive sulphur”. Corrosive sulphur is defined as various forms of organic sulphur compounds (often thermally unstable) such as Cu<sub>2</sub>S, which can cause corrosion of metal parts of the transformer, in particular copper and silver. Dibenzyl disulfide has been found to be the leading corrosive sulphur compound in the insulation oil. This project is focused on finding an effective way to decontaminate such oils. Commonly used transformer oils were purified by sorption technique and by extraction into polar aprotic solvents such as acrylonitrile, dimethyl sulfoxide, N-methyl-2-pyrrolidone or dimethylformamide. The key physico-chemical and chemical properties of transformer oils containing corrosive sulphur were defined. Therefore,



viscosity at 40°C, density at 20°C, contact angle, group composed of transformer oils, distillation curve by simulated distillation, content of sulphur compounds in the oil samples by mass spectrometry (GC/HRMS) and gas chromatograph with chemiluminescence sulphur detector (GC SCD) were determined.



**Tested natural sorbents**

### **Decontamination of brownfields extensively contaminated by organic compounds and heavy metals**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Dekonta, a.s.; supported by TACR, project No. TA04020700)

This project is aimed at finding an optimized solution for soil and groundwater treatment at various brownfield sites. During this project, methods enabling decontamination of premises polluted by a broad range of contaminants, such as petroleum substances, polyaromatic hydrocarbons, or chlorinated and polychlorinated persistent organic pollutants, and heavy metals, will be verified. These techniques will be based on optimized combining of selected physical-chemical processes. Emphases will be put on a treatment train application, comprising adsorption, thermic desorption in aerobic and inert conditions, catalytic incineration, reductive dechlorination, chemical solidification of heavy metals as well as advanced oxidation of water including photocatalytic treatment. Efficiency and economic feasibility of laboratory designed and experimentally tested means of decontamination will be further proven on semipilot and pilot-scale model systems. Technological conclusions will be evaluated on processing of soil from selected brownfields and other contaminated sites in the Czech Republic. Novelty of the proposed project lies in elaboration of a method for separating of heavy metals from gas phase produced during thermal desorption and an algorithm of precisely defined subsequent decontamination methods, which will be verified in practice. The developed algorithm will cover majority of possible pollutant's combinations occurring in brownfields. In the Czech Republic, the problem of brownfields' decontamination in such scope as well as such a comprehensive way has not yet been dealt. [Refs. 7, 11, 20, 28]



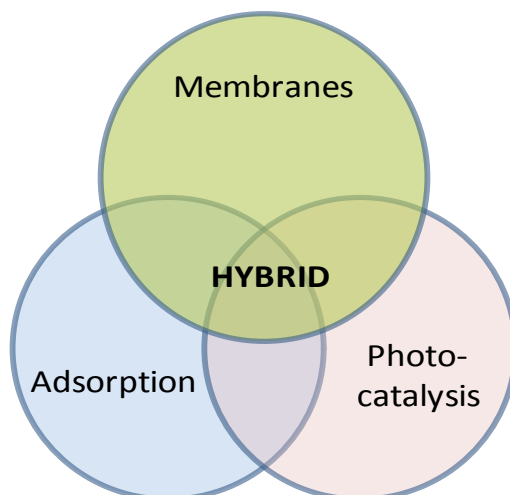


**Laboratory reactor for thermal desorption**

### **Hybride membrane process for water treatment (HYMEPRO)**

(O. Šolcová, L. Matějová (member of the steering group), [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz), [matejova@icpf.cas.cz](mailto:matejova@icpf.cas.cz); joint project with University of Oulu, Lappeenranta University of Technology, Corvinus University of Budapest, National University of Engineering in Lima and 12 industrial partners; supported by Finish funding agency TEKES)

Project deals with the development of a novel, active and sustainable hybrid wastewater treatment process that removes simultaneously heavy metals, arsenic and nutrients from waters. The developed technology is designed based on the green chemistry and engineering principles. [Refs. 13, 21]



### **Production of 3<sup>rd</sup> generation biofuels by enzymatic catalyzed transesterification of microalgal oil**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with EcoFuel Laboratories, TransBiodiesel, Ltd. Israel; supported by MEYS, GESHER/MOST, project No. LJ12002)

The objective of the project is to develop a closed process for autotrophic cultivation of microalgae and biorefinery approach using novel extraction techniques for production of algal

oils and high-value feed additives from wet algal biomass. The oil will be further converted to biodiesel utilizing a novel immobilized enzymatic technology.

Project makes huge benefit from connecting algae cultivation and photo-bioreactor design experience together with the down-stream chemical engineering experience of Czech partners with the complementary experience of Israel partner in the area of biodiesel production. Important benefit lies in the transfer of developed algal biotechnologies to Israel where conditions of warm Mediterranean climate with high level of photosynthetic solar radiation will allow efficient year-round large-scale cultivation of algae mainly using deserted non-arable land for photobioreactors installation. In comparison, climatic conditions in Czech Republic allows for only approx. 150 days cultivation period.

The process consists of cultivation of microalgae in the novel high-rate photobioreactors using waste streams as nutrients, the novel low-energy cell harvesting techniques and lipids extraction directly from wet biomass coupled with advanced high-yield enzymatic transesterification of algal oil into biodiesel. The extraction of oil from algal biomass will be environmentally friendly, leaving residual algal biomass with high content of proteins and carotenoids, suitable for use as animal feed supplement. This biorefinery approach influences positively the feasibility of production of algal biodiesel.

Utilization of vast knowledge of microalgae cultivation techniques and photo-bioreactor existing by partners in Czech Republic will facilitate development of techniques for production of biodiesel feedstock from algal oil. In Israel - TransBiodiesel will contribute to development of non-lipid high tolerance enzymes. Such technologically advanced enzymes will be used in a "pilot unit" for transesterification algal oil using environmentally friendly and energy saving advanced enzymatic process for 3<sup>rd</sup> generation of biodiesel production.

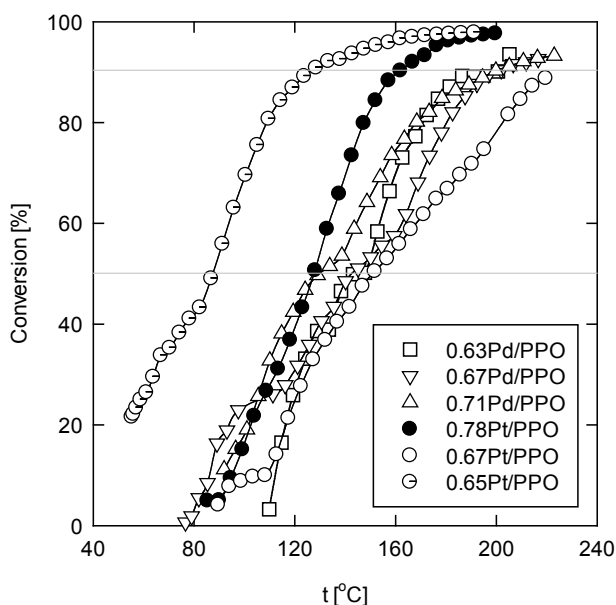
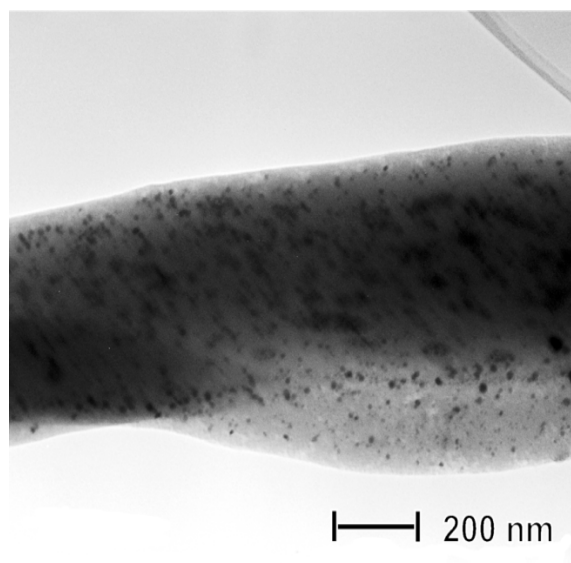


**Pilot plant bioreactor**

### **Washcoated ceramic monoliths for total oxidation of volatile organic compounds**

(P. Topka, [topka@icpf.cas.cz](mailto:topka@icpf.cas.cz); supported by GACR, project No. 13-24186P)

The effect of impregnation method on the size of palladium and platinum nanoparticles supported on poly(2,6-dimethyl-1,4-phenylene) oxide electrospun mats was investigated. Catalysts with similar metal loading (0.63-0.78 wt. %) possessing various mean metal particle size (2.5 – 8.7 nm) were prepared employing different impregnation times and nominal metal loadings. The catalysts were tested in the total oxidation of methanol (1 000 ppm in air). The catalytic performance of platinum catalysts increased with increasing mean size of Pt nanoparticles. On the other hand, the catalytic performance of palladium catalysts did not correlate with the mean nanoparticle size.



**Catalytic performance of platinum and palladium nanoparticles supported on poly(2,6-dimethyl-1,4-phenylene) oxide electrospun mats in the oxidation of methanol**

## International co-operations

Université catholique de Louvain, Louvain-La-Neuve, Belgium: Chlorobenzene oxidation over platinum and gold catalysts

University of Udine, Udine, Italy: Oxidation of model volatile organic compounds over silver, copper and cobalt catalysts

Institute of Catalysis, BAS, Sofia, Bulgaria: New heterogeneous catalysts for environmental protection

University of Liverpool: Theory of chemical bond

Max-Planck Institute for Chemical Physics of Solids, Dresden: Chemical bonding in solids

University of Oulu, Oulu, Finland: New catalysts for VOC oxidation

University of Oulu, Oulu, Finland: Hybrid membrane process for water treatment

University of Poitiers, Poitiers, France: New catalysts for VOC elimination

University of Strasbourg, Strasbourg, France: Determination of transport characteristics of novel materials with hierarchical pore structure

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

Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts

University of Maribor, Maribor, Slovenia: PolyHYPE polymers

University of Graz, Graz, Austria: Porous polymers

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

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

University of Barcelona, Barcelona, Spain: Ion exchanger catalysts

Zhejiang University, Hangzhou, China: Mesoporous poly(divinylbenzenes)

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

University of Bangor, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials

UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification  
University of Udine, Udine, Italy: Characterization of noble metal catalysts and desulfurization on unconventional catalysts  
Istanbul Technical University, Istanbul, Turkey: Synthesis and Thorough Characterization of Composite Functionalized Polymeric Nano-Structure  
Institute of Computational Chemistry, University of Girona, Spain: Computation  
IRD Fuel Cells A/S, Svendborg, Denmark: Fuel cells electroactivity  
Centre National de la Recherche Scientifique, Montpellier, France: Non-carbonaceous supports, catalysts  
FUMA-TECH Gesellschaft für Funktionelle Membranen und Anlagentechnologie MBH, St Ingbert, Germany: Ionomers  
Shanghai Jiao Tong University, Shanghai, China: Ionomers and polymers  
Volvo Technology AB, Göteborg, Sweden: MAE test protocols  
SGL Carbon GmbH, Meitingen, Germany: Electroconductive gas diffusive layers  
JRC Joint Research Centre-European Commission, Brussels, Belgium: FCH tests  
TimCal SA, Bodio, Switzerland: Carbon black supports

## Visitors

A. Spojakina, Institute of Catalysis, BAS, Sofia, Bulgaria  
Dr. Gerardo Cruz, National University of Tumbes, Peru  
Dr. Mónica Gómez, National University of Engineering, Lima, Peru  
L. Benoit, University of Strasbourg, France  
P. Losch, University of Strasbourg, France  
J. Grabowski, Central Mining Institute, Katowice, Poland  
A. Sezai Sarac, Istanbul Technical University Faculty of Sciences  
R. Palcheva, Institute of Catalysis, BAS, Sofia, Bulgaria  
K. Stanczyk, Central Mining Institute, Katowice, Poland  
Y. Zub, Institute of Surface Chemistry NAS, Ukraine  
H. Gao, Shanghai Jiao Tong University, Shanghai, China  
B. Bauer, FUMA-TECH, St Ingbert, Germany  
W. Zhang, FUMA-TECH, St Ingbert, Germany  
D. Jones, Centre National de la Recherche Scientifique, Montpellier, France  
J. Roziere, Centre National de la Recherche Scientifique, Montpellier, France  
J.L. Bonde, IRD Fuel Cells A/S, Svendborg, Denmark  
M. Odgaard, IRD Fuel Cells A/S, Svendborg, Denmark  
M.J. Larsen, IRD Fuel Cells A/S, Svendborg, Denmark  
D.N. Tito, Elysium Projects Ltd., Bangor, United Kingdom  
John Bostock, Elysium Projects Ltd., Bangor, United Kingdom

## Teaching

P. Krystyník: UJEP, Faculty of the Environment, course "Toxicology"  
R. Ponec: CU, Faculty of Science, course "Physical Organic Chemistry"  
O. Šolcová: UCT, Prague, Faculty of Chemical Technology, postgraduate course "Texture of Porous Solids"



## Publications

### Original papers

- [1] Čapek P., Veselý M., Bernauer B., Sysel P., Hejtmánek V., Kočířík M., Brabec L., Prokopová O.: Stochastic Reconstruction of Mixed-Matrix Membranes and Evaluation of Effective Permeability. *Comput. Mat. Sci.* 89, 142-156 (2014).
- [2] Čapek P., Veselý M., Hejtmánek V.: On the Measurement of Transport Parameters of Porous Solids in Permeation and Wicke-Kallenbach Cells. *Chem. Eng. Sci.* 118, 192-207 (2014).
- [3] Dytrych P., Klusoň P., Dzik M., Veselý M., Morozová M., Sedláková Z., Šolcová O.: Photo-Electrochemical Properties of ZnO and TiO<sub>2</sub> Layers in Ionic Liquids Environment. *Catal. Today* 230, 152-157 (2014).
- [4] Dytrych P., Klusoň P., Slater M., Šolcová O.: Theoretical Interpretation of the Ionic Liquid Phase Role in the (R)-Ru-BINAP Catalyzed Hydrogenation of Methylacetoacetate. *React. Kinet. Mech. Cat.* 111(2), 475-487 (2014).
- [5] Guilera J., Hanková L., Jeřábek K., Ramírez E., Tejero J.: Influence of the Functionalization Degree of Acidic Ion-Exchange Resins on Ethyl Octyl Ether Formation. *React. Funct. Polym.* 78, 14-22 (2014).
- [6] Hanková L., Holub L., Meng X., Xiao F.-S., Jeřábek K.: Role of Water as a Coporogen in the Synthesis of Mesoporous Poly(divinylbenzenes). *J. Appl. Polym. Sci.* 131(23), 41198 (2014).
- [7] Hejda S., Drhová M., Křišťál J., Buzek D., Krystyník P., Klusoň P.: Microreactor as Efficient Tool for Light Induced Oxidation Reactions. *Chem. Eng. J.* 255, 178-184 (2014).
- [8] Krýsa J., Baudys M., Zlámal M., Krýsová H., Morozová M., Klusoň P.: Photocatalytic and Photoelectrochemical Properties of Sol-Gel TiO<sub>2</sub> Flms of Controlled Thickness and Porosity. *Catal. Today* 230, 2-7 (2014).
- [9] Krystyník P., Klusoň P., Hejda S., Bůžek D., Mašín P., Tito D.N.: Semi-pilot Scale Environment Friendly Photocatalytic Degradation of 4-Chlorophenol with Singlet Oxygen Species - Direct Comparison with H<sub>2</sub>O<sub>2</sub>/UV-C Reaction System. *Appl. Catal., B* 160-161, 506-513 (2014).
- [10] Krystyník P., Klusoň P., Hejda S., Mašín P., Tito D.N.: A Highly Effective Photochemical System for Complex Treatment of Heavily Contaminated Wastewaters. *Water Environ. Res.* 86(11), 2212-2220 (2014).
- [11] Kuráň P., Trögl J., Nováková J., Pilařová V., Dáňová P., Pavlorková J., Kozler J., Novák F., Popelka J.: Biodegradation of Spilled Diesel Fuel in Agricultural Soil: Effect of Humates, Zeolite, and Bioaugmentation. *Sci. World J.* 2014, ID 642427 (2014).
- [12] Losch P., Boltz M., Soukup K., Song I.-H., Yun H.-S., Louis B.: Binderless Zeolite Coatings on Macroporous  $\alpha$ -SiC Foams. *Micropor. Mesopor. Mat.* 188, 99-107 (2014).
- [13] Matěj Z., Kadlecová A., Janeček M., Matějová L., Dopita M., Kužel R.: Refining Bimodal Microstructure of Materials with MSTRUCT. *Powder Diffr.* 29(Suppl. 2), S35-S41 (2014).
- [14] Sevšek U., Brus J., Jeřábek K., Krajnc P.: Post-polymerisation Hypercrosslinking of Styrene/divinylbenzene poly(HIPE)s: Creating Micropores within Macroporous Polymer. *Polymer* 55(1), 410-415 (2014).
- [15] Soukup K., Hejtmánek V., Stanczyk K., Šolcová O.: Underground Coal Gasification: Rates of Post Processing Gas Transport. *Chem. Pap.* 68(12), 1707-1715 (2014).
- [16] Soukup K., Hejtmánek V., Šolcová O.: Evaluation of Mass Transport Properties of the Advanced Medical-Interesting Porous Solids. *WSEAS Transactions on Heat and Mass Transfer* 9, 102-110 (2014).
- [17] Soukup K., Topka P., Hejtmánek V., Petráš D., Valeš V., Šolcová O.: Noble Metal Catalysts Supported on Nanofibrous Polymeric Membranes for Environmental Applications. *Catal. Today* 236, 3-11 (2014).
- [18] Sterchele S., Centomo P., Zecca M., Hanková L., Jeřábek K.: Dry- and Swollen-State Morphology of Novel High Surface Area Polymers. *Micropor. Mesopor. Mat.* 185, 26-29 (2014).
- [19] Šolcová O., Balkan T., Guler Z., Morozová M., Dytrych P., Sarac S.: New Preparation Route of TiO<sub>2</sub> Nanofibers by Electrospinning: Spectroscopic and Thermal Characterizations. *Sci. Adv. Mater.* 6(12), 2618-2624 (2014).

- [20] Šolcová O., Topka P., Soukup K., Jiráková K., Váňová H., Kaštánek F.: Solid Waste Decontamination by Thermal Desorption and Catalytic Oxidation Methods. *Chem. Pap.* 68(9), 1279-1282 (2014).
- [21] Valeš V., Matějová L., Matěj Z., Brunátová T., Holý V.: Crystallization Kinetics Study of Cerium Titanate  $CeTi_2O_6$ . *J. Phys. Chem. Solids* 75(2), 265-270 (2014).
- [22] Vít Z., Gulková D., Kaluža L., Boaro M.: Effect of Catalyst Precursor and Its Pretreatment on the Amount of  $\beta$ -Pd Hydride Phase and HDS Activity of Pd-Pt/Silica-Alumina. *Appl. Catal. B-Environ.* 146(SI), 213-220 (2014).
- [23] Vít Z., Kaluža L., Gulková D.: Comparison of Nitrogen Tolerance of PdMo/Al<sub>2</sub>O<sub>3</sub> and CoMo/Al<sub>2</sub>O<sub>3</sub> Catalysts in Hydrodesulfurization of Model Compounds. *Fuel* 120, 86-90 (2014).
- [24] Žáček P., Kaluža L., Karban J., Storch J., Sýkora J.: The Rearrangement of 1-Methylcyclohex-1-ene during the Hydrodesulfurization of FCC Gasoline over Supported Co(Ni)Mo/Al<sub>2</sub>O<sub>3</sub> Sulfide Catalysts: the Isolation and Identification of Branched Cyclic C<sub>7</sub> Olefins. *React. Kinet. Mech. Cat.* 112(2), 335-346 (2014).
- [25] Žebrák R., Mašín P., Klusoň P., Krystyník P.: Using of Photochemical H<sub>2</sub>O<sub>2</sub>/UVC Decontamination Cell for Heavily Polluted Waters. *Waste Forum* 2014(2), 55-62 (2014).

### Chapters in books

- [26] Ponec R.: Late Reminiscence of Unexplored Scientific Links with Ante. Parity of Kekulé Structures and Algebraic Structure Count. In: *Ante Graovac - Life and Works*. (Gutman, I.- Pokric, B.- Vukicevic, D., Ed.), pp. 243-258, University of Kragujevac, Kragujevac 2014.

### Patents

- [27] Kaštánek F., Šolcová O., Maléterová Y., Spáčilová L., Maternová H., Mašín P., Žebrák R.: Zařízení pro fotokatalytickou dekontaminaci vod s obsahem organických látek, zejména endokrinních disruptorů. Device for Photo-Catalytic Decontamination of Water Containing Organic Compounds, Especially Endocrine Disruptors. *Pat. No. 304681/PV* 2013-522. Applied: 13.07.03, Patented: 14.07.17.
- [28] Váňová H., Raschman R., Kukačka J., Šolcová O., Topka P., Jiráková K., Veselý J.: Způsob dekontaminace zeminy a zařízení k provádění způsobu. Soil Decontamination Method and Apparatus for Performing the Method. *Pat. No. 304461/PV* 2012-670. Applied: 12.09.27, Patented: 14.04.02.