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Fields of research

- Advanced catalytic oxidation processes
- Catalytic combustion of volatile organic compounds in waste gases
- Catalytic decomposition of N₂O
- 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; 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.

During the UCG process as well as a long time after the process termination a great number of hazardous environmental contaminants (both inorganic and organic species) can be released into the groundwater environment. Within this project, the solute transport processes in groundwater were modeled using the saturated zone model of groundwater flow including phenomena that incorporates advection, both mechanical and hydrodynamic dispersion, solute diffusion as well as adsorption of solutes on the rock inner surfaces. Used model was formulated under consideration of the rock saturation with water. Water fills completely all volume of voids in porous rocks and creates a saturation zone. From a mathematical point of view, the model description takes into consideration Darcy's law, Fick's law of diffusion and equation of adsorption isotherms.

Fly ash from coal combustion have been chosen as potentially best fill material for filling of UCG voids and control of release and migration of contaminants due their widely known ability to isolate contaminants, between other in landfilling, beneficial physical properties and availability. From the point of the view of isolation of contaminants a very important factor is the filtration coefficient of solidified (stabilized) fly ash – water mixtures, what become subject of laboratory measurements. [Ref. 39]



Detail of reactor filled up by sand with the prepared slot for sorbents

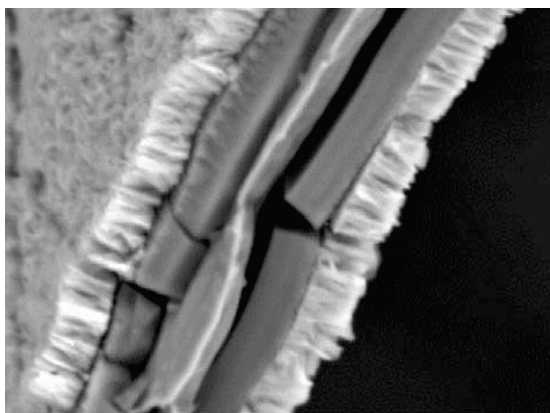
Structured catalysts with low concentration of active components for total oxidation of VOC

(K. Jirátová, jiratova@icpf.cas.cz; joint project with ICT and IIC; supported by GACR, project No. 106/10/1762)

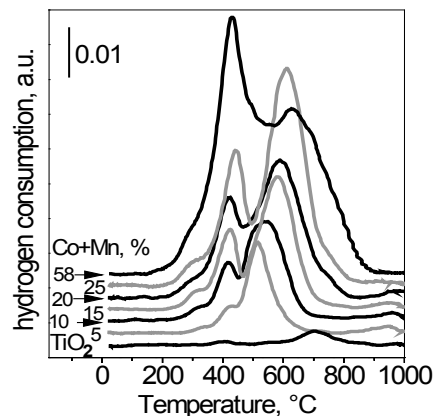
Oxide catalysts containing various combinations of Cu, Co, Ni, Mn, and Al, grained or supported on oxidized aluminum foil $\text{Al}_2\text{O}_3/\text{Al}$, were studied in terms of their chemical and physical properties, and activity in total ethanol oxidation. Ternary co-precipitated catalysts in the form of grains obtained from layered double hydroxide-like precursors were highly active, especially those containing manganese. Deposition of the selected precursors on an anodized aluminum foil-support afforded less active catalysts, mainly because the required metal molar ratios were not achieved, and insufficient metal amounts were deposited. However, by controlling the preparation conditions (pH), higher loading of active components and higher catalytic activity were obtained.

Catalytic activity of the Co-Mn-Al mixed oxide catalyst (Co:Mn:Al molar ratio of 4:1:1) supported over titania was examined in total oxidation of ethanol. The catalysts activity gradually increased with increasing active phase content. Low concentration of Co-Mn-Al oxides in the catalyst negatively affected formation of reaction byproducts: carbon monoxide production steeply increased when Co+Mn metals concentration were lower than 5 wt. %. On the other hand, formation of the second main reaction intermediate, acetaldehyde was limited, when acidity of the catalyst was not high, i.e. concentration of Co+Mn metals over titania was low.

Physical-chemical properties of the catalysts containing precious metals, like reducibility, acidity, basicity, and of metal specific surface area were also studied. [Refs. 20, 21, 26, 30, 31]



Scanning electron microscope image of an LDH-type Co-Mn-Al precursor grown on an $\text{Al}_2\text{O}_3/\text{Al}$ support



Temperature programmed reduction curves of the supported Co-Mn-Al catalysts having various amounts of active components (Co+Mn) on titania

Removal of heavy metals and radionuclides from water using ceramic membranes

(O. Šolcová, 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.

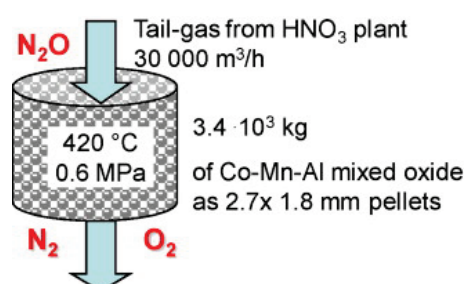
Therefore, the main objective of the project is to develop a family of advanced nanofiltration (NF) and UF ceramic composite membranes containing functionalized mesoporous silica layers which will be capable of selective binding of heavy metals (Hg, Cd, Cr) and uranium from surface and waste waters and thus preventing or minimizing the environmental exposure to hazardous substances. [Refs. 37, 38]

Abatement of N₂O emissions in off-gas from nitric acid technology

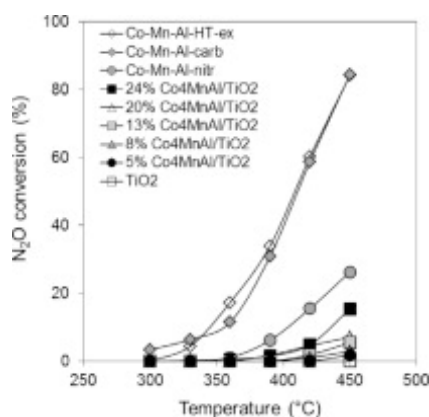
(K. JirátoVá, jiratova@icpf.cas.cz; joint project with TU of Ostrava, and ICT; supported by TACR, project No. TA01020336)

Pilot reactor for low temperature N₂O decomposition in off-gases from HNO₃ production was designed. Pseudo-homogeneous one-dimensional model of an ideal plug flow reactor was used for modeling of N₂O decomposition in a laboratory fixed bed reactor filled with grains or pellets of a Co–Mn–Al mixed oxide catalyst. Increase in inlet pressure up to 0.6 MPa did not influence the effective diffusion coefficient, but improved the achieved N₂O conversion. Based on the laboratory data of N₂O decomposition over Co–Mn–Al mixed oxide pellets, catalyst bed of 3400 kg was estimated for target 90% N₂O conversion (30 000 m³ h⁻¹ of exhaust gases from HNO₃ plant containing 0.1 molar% N₂O, 0.01 molar% NO, 0.01 molar% NO₂, 3 molar% H₂O, 5 molar% O₂) at 420°C and 600 kPa inlet pressure.

A series of Co–Mn–Al/TiO₂ catalysts with different Co+Mn loading (5–24 wt. %) was prepared by impregnation of TiO₂ support and compared with bulk Co–Mn–Al mixed oxides. TiO₂ acted only as a catalytic support and did not contribute to the catalytic activity. The N₂O conversion over TiO₂-supported Co–Mn–Al catalysts was increasing with Co + Mn loading, and was proportional to the amount of easily reducible components. Comparing the catalysts with identical amount of active components, the highest catalytic activity was achieved on the calcined precursors having carbonates in their molecules (layered double hydroxides Co–Mn–Al-HT-ex and Co–Mn–Al-carb), the lowest one on the calcined Co–Mn–Al nitrates due to the lower surface area, less advantageous porous structure and worse reducibility. [Refs. 12, 27]



Scheme of the reactor arrangement for N₂O decomposition



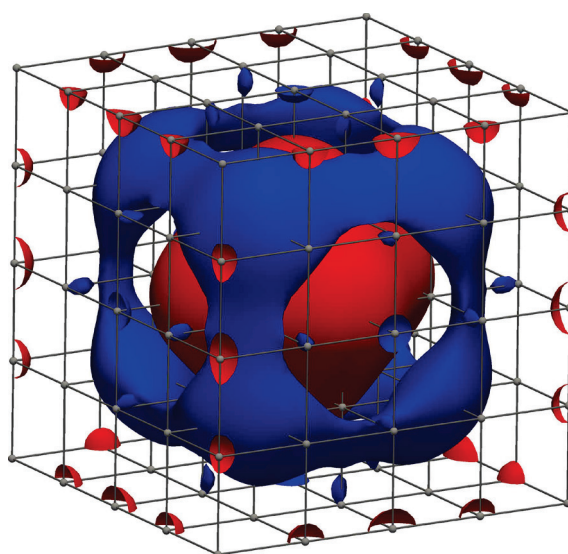
Temperature dependence of N₂O conversion over Co–Mn–Al mixed oxide supported on TiO₂. Conditions: 0.1 mol % N₂O balanced in He, 0.1 MPa, GHSV = 60 l g⁻¹ h⁻¹

Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, rponec@icpf.cas.cz; joint project with University of Pécs, Hungary, University of Girona, Spain; supported by GACR, project No. 203/09/0118)

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 behavior 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 bonds. Especially useful in this respect were found the approaches known as the analysis of domain averaged Fermi holes (DAFH) and the generalized population analysis (GPA). These approaches have been applied to the elucidation of electron reorganization during the carbocationic rearrangements involved in the biosynthesis of terpenes and important new insights were also obtained from the generalization of the DAFH analysis for the description of the bonding interactions in solids.

[Refs. 1, 8]

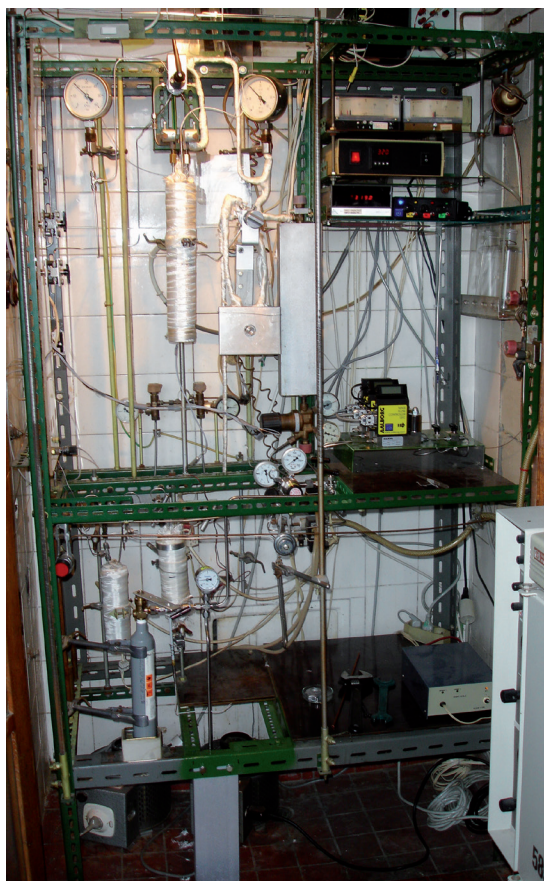


**DAFH orbital from the DFT calculation for the cubic hydrogen lattice.
The isosurface of the orbital amplitude 0.0107 are colored with the orbital sign.
The basin of the corresponding DAFH is located in the middle of the region**

Study of hydrodesulfurization and its inhibition by hydrogenation (denitrogenation) over catalysts containing small amounts of noble metals

(Z. Vít, vít@icpf.cas.cz; joint project with Department of Chemistry, Physics and Environment, University of Udine, Italy; supported by GACR, project No. 104/09/0751)

Modification of mesoporous silica-alumina by nitric acid extraction was used for preparation of catalysts with a conventional CoMoS phase. Extraction of support significantly increased its BET surface area and protonic acidity, which both positively influenced the hydrodesulfurization (HDS) activity of catalysts. This is because of leaching of non-acidic aluminum oxide which blocks the strong acidic tetrahedral Al-OH-Si sites. Protonic acidity of catalysts was evaluated by means of tests in skeletal isomerization of cyclohexene and cracking of cumene. On the other hand, acid extraction diminished the amount of deposited Mo phase. It was found that the higher dispersion of active phase and specific activities in benzothiophene HDS were achieved on samples synthesized from the modified supports. An interesting point is that the catalysts keep the strong protonic acidity also after deposition of the CoMoS phase.

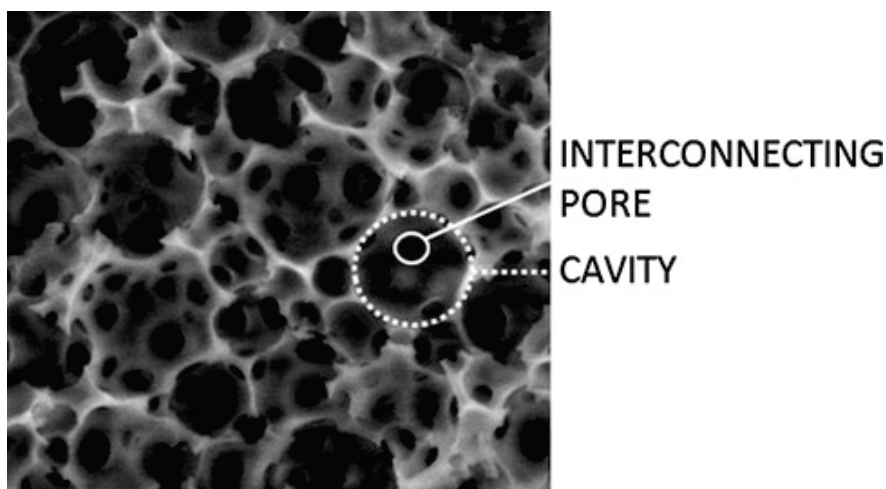


Pressure flow microreactor with fixed bed of catalyst for hydrodesulfurization

Post-polymerization hypercrosslinking of monolithic polymers

(K. Jeřábek, kjer@icpf.cas.cz; joint project with University of Maribor, Slovenia; supported by MEYS, project No. MEB091107)

Within this project are investigating possibilities of modifications of morphology of monolithic PolyHIPE porous polymers by additional crosslinks introduced to the already polymerized monolithic material. In this manner, much smaller pores are created thus significantly enlarging the surface area while leaving the larger pores intact. [Ref. 29]

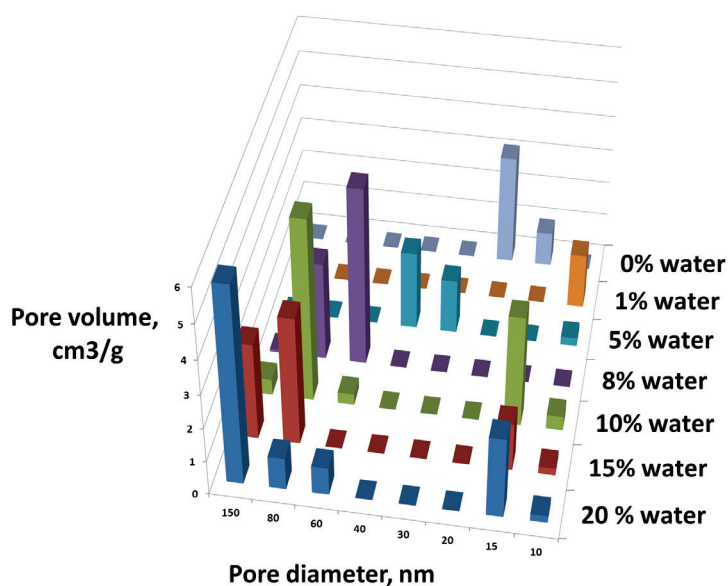


SEM picture showing typical structure of PolyHIPE monolith

Morphology and application properties of mesoporous poly(divinylbenzenes)

(K. Jeřábek, 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. 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 and applications for which the exceptional properties of the mesoporous functional polymers could be advantageous. [Ref. 16]

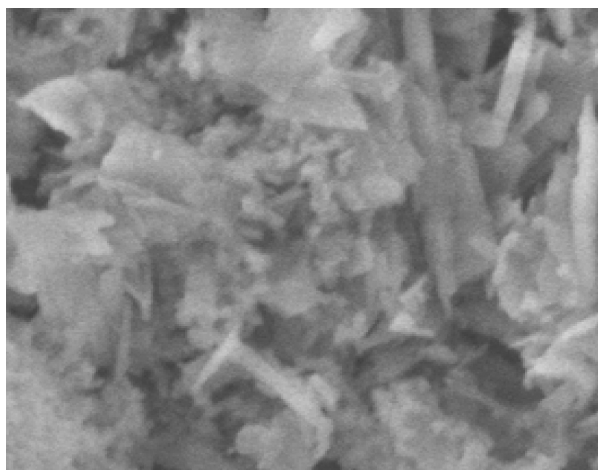


Dependence of swollen-state morphology of poly(divinylbenzenes) on water presence in the porogenic solvent

New catalysts for VOC oxidation

(P. Topka, topka@icpf.cas.cz; joint project with Department of Process and Environmental Engineering, University of Oulu, Finland; supported by ASCR, project No. M200720901)

Commercial VOC oxidation catalysts can be used as comparative materials during development of new or improved catalysts. The objective of this study was to investigate physicochemical properties of EnviCat[®] commercial catalysts and their performance in total oxidation of three model compounds (dichloromethane, toluene and ethanol) at laboratory scale. The reactivity of model volatile organic compounds was decreasing in the order ethanol > toluene > dichloromethane. The Cu–Mn/Al catalyst was found to be the most active and selective catalyst in ethanol oxidation. In oxidation of dichloromethane, the Pt–Pd/Al–Ce catalyst with 0.10 wt. % Pt + Pd was the most active, while the most selective one (giving the highest HCl yield) was the Pt–Pd/Al catalyst containing 0.24 wt. % Pt + Pd. In toluene oxidation, the Pt–Pd/Al catalyst with 0.24 wt. % Pt + Pd possessed the highest activity; the selectivity to CO₂ was 100 % for all investigated catalysts. Obtained results showed that the performance of commercial catalysts in laboratory scale tests can be different from that declared by catalyst supplier. A possible difference in catalytic performance at industrial and laboratory scale should be taken into account when industrial catalysts are used in laboratory scale tests. [Ref. 25]

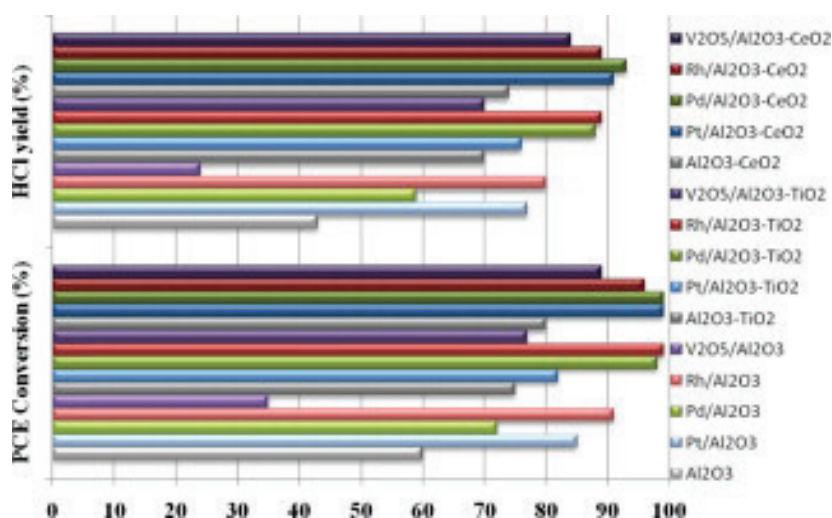


Surface of Envicat® VOC-1544 catalyst as seen by field-emission scanning electron microscope

Development of oxide catalysts for total oxidation of ethanol

(J. Gaálová, gaalova@icpf.cas.cz; supported by GACR, project No. 106/10/P019)

Pt, Pd, Rh and V_2O_5 metallic monolithic catalysts supported on Al_2O_3 , $Al_2O_3-CeO_2$ and $Al_2O_3-TiO_2$ were examined in the oxidation of perchloroethylene. To ensure high HCl yields, the amount of water as a hydrogen source was optimized to be 1.5 wt. % by testing the effect of water content on perchloroethylene oxidation. Water not only enhanced the selectivity towards HCl formation but also improved the perchloroethylene oxidation to some extent. Both activity and selectivity of the catalysts were found to be related to the properties of the catalyst support; addition of TiO_2 or CeO_2 into Al_2O_3 enhanced catalysts' efficiency regardless of the active phase. Pt, Pd and Rh catalysts showed high catalytic activity, perchloroethylene conversions ranging from 72% to 99%, and HCl yields from 59% up to 93% were observed. Both activity and selectivity of the Pt/ $Al_2O_3-CeO_2$ and Pd/ $Al_2O_3-CeO_2$ catalysts were superior to the other tested catalysts. The results show that in the oxidation of perchloroethylene, the redox properties of the catalyst and the amount of activated oxygen may play bigger role than the acidity. To confirm the suspected positive effect on perchloroethylene oxidation coming from the bidisperzed mesopores seen over ceria-doped catalysts needs further testing. [Refs. 31, 32]

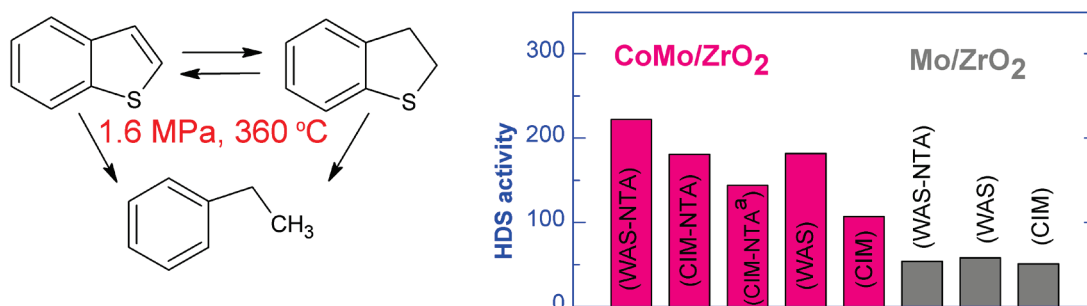


Conversion of perchloroethylene and yield of HCl achieved over investigated catalysts

Unconventional composition and preparation of sulfide hydrotreating catalysts

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

The principles of the use of chelating agents such as nitrilotriacetic acid (NTA) were studied for our original preparation methodology. It was found that the employing of NTA during preparation of CoMo catalysts supported on the monoclinic ZrO₂ increased the hydrodesulfurization (HDS) activity within the range 22–69 %. The molar ratio NTA/(Co+Mo) to achieve high HDS activities was 1/1. The most active CoMo/ZrO₂ catalyst was prepared by the impregnation of the support from the solution made by dissolution of MoO₃, CoCO₃ and NTA in water followed by sulfidation without previous calcination. Furthermore, the new alumina-supported NiMo hydrodesulfurization catalysts have been prepared by loading the Anderson-type nickel heteropolyoxomolybdate on the alumina initially modified with nickel, cobalt or boron. Nickel incorporation in the alumina prior to loading (molar ratio of the total amount Ni in the catalysts is Ni/(Mo+Ni) = 0.24) resulted in an activity for 1-benzothiophene HDS that was nearly twice as much as the activity observed for the unmodified, B- and Co modified catalysts. The new mesoporous silica-alumina (SA) was modified by acid leaching and studied as an alternative support for Mo and CoMo catalysts for HDS of benzothiophene, cyclohexene isomerization and cumene cracking. Progressive leaching of the parent SA containing 52 wt. % Al₂O₃ (SA52) led to decrease of Al₂O₃ content (33 and 19 wt. % in MSA33 and MSA19 support, respectively). This decrease was accompanied with an increase of the surface area and exposition of strong acidity. [Refs. 6, 9-11, 28]

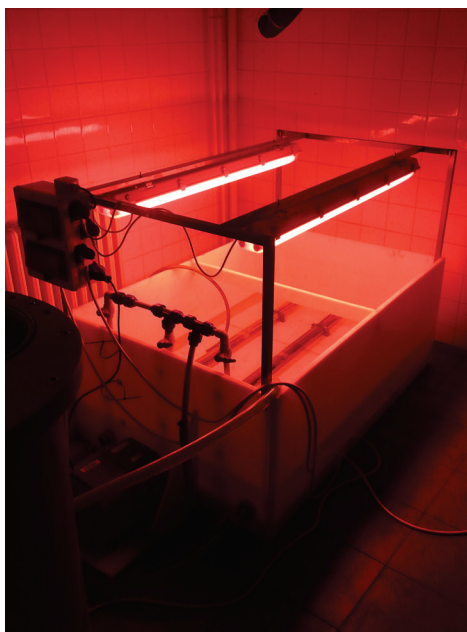


The activity of new CoMo catalysts in hydrodesulfurization of 1-benzothiophene

Reactive chemical barriers for decontamination of heavily polluted waters

(P. Klusoň, kluson@icpf.cas.cz; joint project with Dekonta a.s.; supported by MIT, project No. FR-TI1/065)

The project, which will be finished in May 2013, is now focusing on the final studies of the special oxidations of contaminants in industrially polluted waters. Special attention was paid to aniline and nitrobenzene waters, to waters with dissolved chlorinated compounds and to inorganic contamination with certain specific ions. The used methods were again the photocatalytic oxidations with phthalocyanines, name with Zn phthalocyanine, and with UVC and hydrogen peroxide. Among other techniques electrocoagulation was also tested to reduce both the organic as well as the inorganic pollutants. The project thus deals in a complex manner with the problem of industrial pollution of various types and origins. The Recheba concept represents a kind of passive approach, however, assisted with highly advanced processes for effective water decontamination. The systems had been still tested on a laboratory scale, however, much more attention was now paid to the large scale operations.

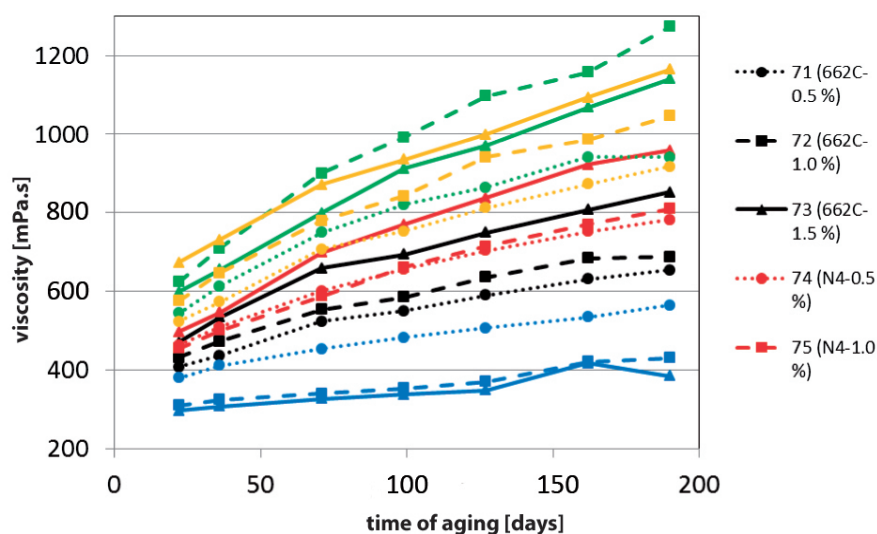


Detail of the phthalocyanine decontamination unit

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

(P. Klusoň, 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 tetraalkylammonium 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.



Viscosity change (at $T = 23^{\circ}\text{C}$) in time of alkyde resin with various ionic liquids at three concentrations (additives do not change the Newtonian character of resin)

Composed molecular templates for preparation of assembled functional nanoparticles

(P. Klusoň, kluson@icpf.cas.cz; joint bilateral project with Bangor University, School of Chemistry, Wales, UK; supported by ASCR, project No. M200720904)

This project was finished in March 2012 and it was focusing on making smart functional structures and systems based on template nanoparticles. Among many methods, bottom-up approaches involving templates have dominated for the preparation of one-dimensional or multidimensional nanostructures. This pathway is particularly useful if precise replication is achieved in the nanometer precision. It corresponds to the assembly of well-defined nanobuilding blocks consisting of perfectly calibrated objects keeping their integrity in the final material. In the last project period also ionic liquids were used as molecular patterns and tools for imprinting the structure to the forming nanoparticles. [Refs. 40, 43]

Utilization of combined thermal desorption and catalytic oxidation methods for solid waste decontamination

(O. Šolcová, solcova@icpf.cas.cz; joint project with Dekonta a.s.; supported by MIT, project No. FR-TI1/059)

Project develops and verifies a new technology for decontamination of solid waste containing toxic organic substances, which is based on treatment of the waste by thermal desorption process and subsequent catalytic oxidation of desorbed organic contaminants. Research activities aimed at solution of some technical problems related to full-scale application of the developed technology will be realized together with testing under real conditions.

The combined thermal desorption and catalytic oxidation unit for the soil decontamination was studied at the pilot plant scale. To guarantee flowing of the exhaust gas from the thermal desorption unit into the catalytic oxidation unit the Venturi pump was applied. After the thermal desorption process no residual concentration of contaminants in the soil were detected. Although the contaminant concentrations at the inlet of the catalytic reactor significantly varied during experiments, the efficiency of catalytic oxidation was higher than 90 % in all cases. [Ref. 42]



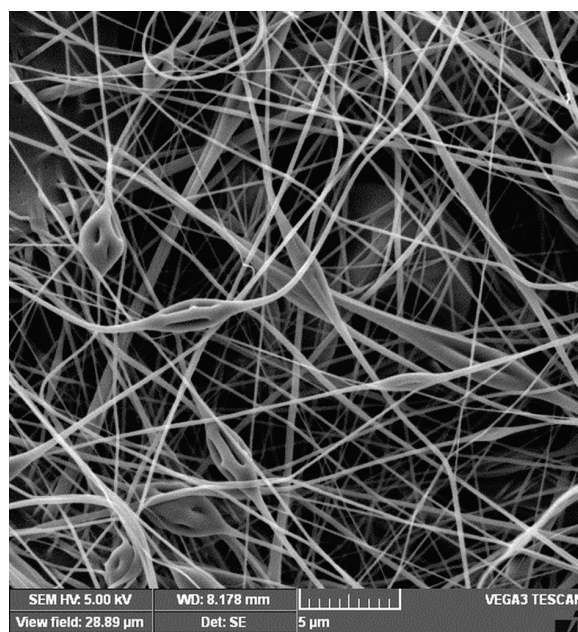
The combined thermal desorption and catalytic oxidation unit

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; joint project with CU and JH IPC; supported by GACR, project No. P204/11/1206)

Searching after the functional relationship between diffusion of fluid in disordered solids (e.g. porous solids) and their microstructure is an active field of research in membrane science, catalysis, biophysics, civil engineering and other branches of research and development. During several past decades the pulsed field gradient (PFG) NMR technique has proved to be a powerful tool for measuring of self-diffusion in such systems. The focus of the project is on transport investigation of liquid species contained in porous materials (non-consolidated and consolidated) with monodisperse and bidisperse porous structure with excursions to adjacent supercritical regions. A rational system of transport-related structure characteristics to predict transport behavior of liquids and supercritical fluids will be searched by combined application of PFG NMR, image analysis of porous materials and molecular simulation of self-diffusion in selected two-phase systems.

The transport parameters of some porous samples of nanofibrous membranes based on poly(2,6-dimethyl-1,4-phenylene oxide) prepared by electrospinning technology were evaluated. The steady-state counter-current diffusion method was adapted for such type of samples (ultrathin slices of very permeable material, approximately 80% porosity). The special apparatus is able to perform binary diffusion experiments at low-pressure (10–60 kPa). The Knudsen number has a convenient value in this pressure region and the mean free paths of molecules are longer. This fact takes a reasonable effect for transport parameters of macroporous material determination, their precision and confidence. At the same time, the new data evaluating software (boundary value problem connected with parameter optimization by the simplex method) was designed for the transport parameters calculation. Resulting from this approach, the confidence limits for the calculated transport parameters could be determined by the better way. The transport parameter values were compared with their counterparts obtained by other method – quasi-steady permeation. The steady-state diffusion method processed under low pressure conditions appears as a suitable method for characterization of the quasi-uniform macroporous materials. [Ref. 34]



SEM image of the parent nanofibrous support

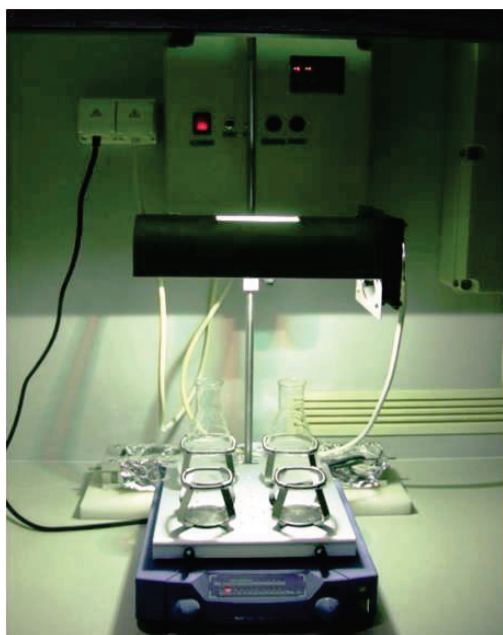
Removal of endocrine disruptors from waste and drinking water by photocatalytic and biological processes

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

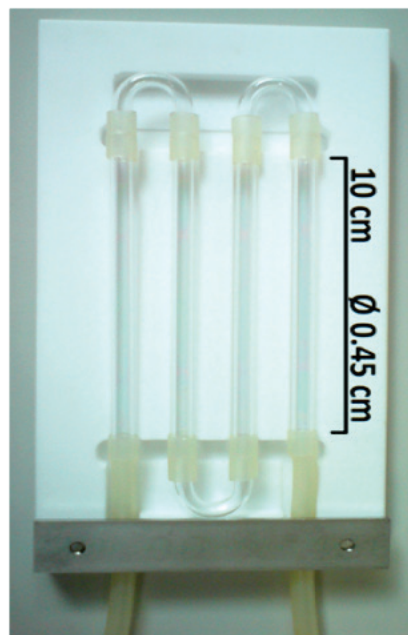
The necessity to find alternative solutions for environmental protection leads to the development and use of the new technologies. Photo-catalysis using semiconductor oxides have found an increasing interest to solve the global pollution problems. Compared to the other photo-catalysts TiO_2 (and/or doped TiO_2) seems to be the most promising material not only in advanced oxidation photo-catalytic processes (AOP). It is well established that titanium oxide and related nanostructure materials in the presence of UV light (in dependence on conditions also in the presence of visible-light) can create very active species that are able to restore and preserve a clean environment by decomposing harmful organics; killing bacteria and viruses and being easily self-cleaned. Our investigation insists on the photo-catalyst immobilization in the form of a thin film trying to improve the efficiency of photocatalytic processes. 17α -ethynylestradiol belongs to the group of the environmental estrogens that act as the hormonal system of the body. Its effect is desirable, especially in hormonal contraception.

The degradation of 17α -ethynylestradiol was measured in the batch and continuous photocatalytic reactors. Initial concentration of ethynylestradiol was in the range 20 to 25 ppm in batch reactor and 11 to 14 ppm in the continuous flow reactor. Four various flow rates (2 ml/min, 1 ml/min, 0.4 ml/min and 0.2 ml/min) were used for degradation of ethynylestradiol in the continuous arrangement. As photocatalyst, TiO_2 thin layers on the glass beads and glass tubes under UV light were applied. 17α -ethynylestradiol degradation activity and selectivity were compared for both arrangements with respect to the possible application.

During the degradation process the estrogenic activity decreased from 97 % to 3 %. Values of the estrogenic activity correspond with decrease of 17α -ethynylestradiol concentration. Conversion of 17α -ethynylestradiol (EE2) achieved 94 % after eight hours. No enhanced toxicity was detected during the experiment that stayed at the zero level. [Refs. 14, 15, 18, 26, 35]



Batch photo-reactor



Plug flow microphoto-reactor

Ionic liquids as additives for special pigments

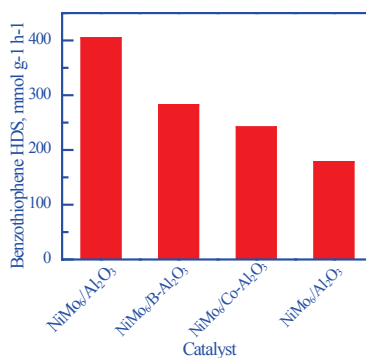
(O. Šolcová, solcova@icpf.cas.cz; joint project with Synthesia, Techem; supported by MIT, project No. FR-TI4/189)

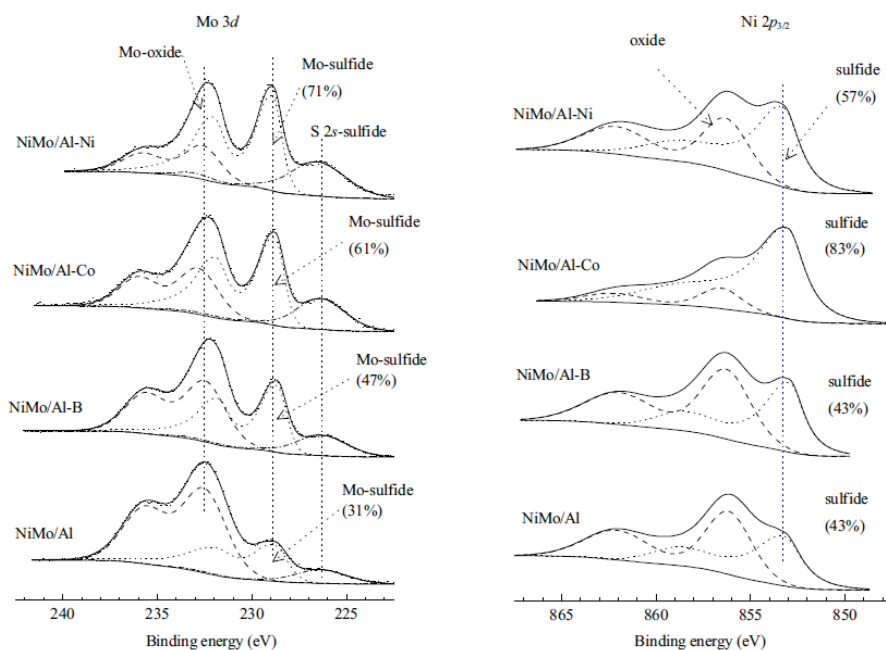
Ionic liquids are composed of large ions with a low degree of the overall molecular symmetry. Very high coulombic interactions are behind their impressive electrical and mechanical stabilities, thermal and pressure resistivity, and extremely low tension of vapors. Low flammability, very good electrical 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-triethylammonium 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.

New heterogeneous catalysts for environmental protection

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

A hydrotreating NiMo/ γ -Al₂O₃ catalyst (12 wt.% Mo and 1.1 wt. % Ni) was prepared by impregnation of the support with the Anderson-type heteropolyoxomolybdate (NH₄)₄Ni(OH)₆Mo₆O₁₈. Before impregnation of the support, it was modified with an aqueous solution of H₃BO₃, Co(NO₃)₂, or Ni(NO₃)₂. The catalysts were investigated using N₂ adsorption, O₂ chemisorption, X-ray diffraction, UV-Vis spectroscopy, Fourier transform infrared spectroscopy, temperature-programmed reduction, temperature-programmed desorption, and X-ray photoelectron spectroscopy. The addition of Co, Ni, or B influenced the Al₂O₃ phase composition and gave increased catalytic activity for 1-benzothiophene hydrodesulfurization (HDS). X-ray photoelectron spectroscopy confirmed that the prior loading of Ni, Co or B increased the degree of sulfidation of the NiMo/ γ -Al₂O₃ catalysts. The highest HDS activity was observed with the NiMo/ γ -Al₂O₃ catalyst with prior loaded Ni. TiAlZr mixed oxides, synthesized using sol-gel method, were characterized and used as supports of HDS catalysts prepared by impregnation either with molybdenum heteropolyacid or its cobalt salt. No formation of a new oxide phase was revealed in the synthesized mixed materials. Incorporation of cobalt into the catalyst masked the effect of the support composition. [Refs. 10, 17, 28]



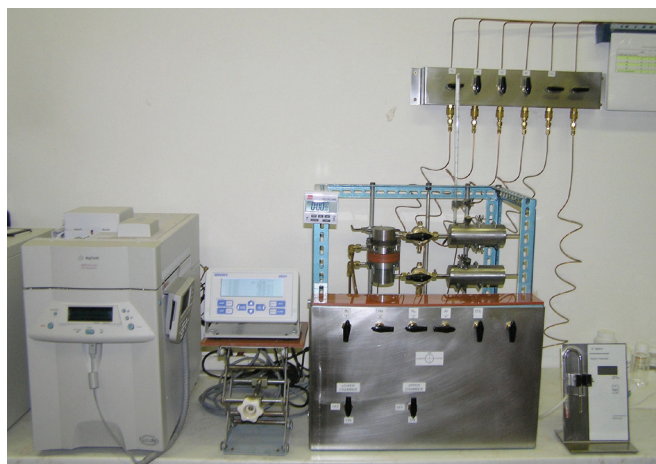


The preparation of CoMo catalysts using Anderson-type heteropolyoxomolybdate: effect of Al₂O₃ modification on benzothiophene HDS and XPS patterns

Transport characteristics of novel biocompatible materials

(K. Soukup, soukup@icpf.cas.cz; supported by GACR, project No. P106/11/P459)

The development and design of advanced bioactive and biocompatible porous materials for medical applications requires a thorough understanding of the texture and transport properties impact on their clinical efficiency. The project is focused on mass transport measurements and the transport characteristic determination of biocompatible clinical valuable materials consisted of nanofibrous mats/membranes prepared by electrospinning technique, hydroxyapatite and apatite. Transport characteristics are determined in liquid/solid as well as gas/solid systems by combination of inverse liquid chromatography and Graham's diffusion cell methods. Effective diffusion coefficients in liquid phase are evaluated using a method based on the fitting of a set of experimental chromatographic profiles to the Kubin-Kučera model. Fitting of the gas diffusion data obtained from Graham's diffusion cell to the Mean Transport-Pore Model provide transport characteristics. The obtained transport parameters are compared with characteristics from the standard textural analyses. [Ref. 33]

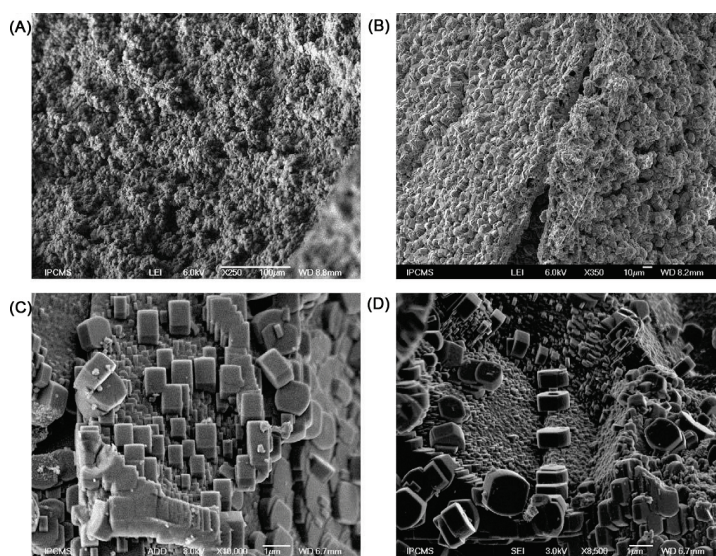


Graham's diffusion cell setup

Novel materials with hierarchical pore structure: preparation and evaluation of the transport characteristics

(K. Soukup, soukup@icpf.cas.cz; joint bilateral project with University of Strasbourg; supported by MEYS, project No. 7AMB12FR029)

In the present bilateral project, we would like to propose strategies towards the design of structured catalytic beds made of hierarchical zeolites with improved hydrodynamics (compared to extrudates or conventional pellets), combining both the advantages of zeolitic catalysts and of a tailored porosity (triple level of porosity: micro-, meso- together with an appropriate macroporosity). In order to prepare material with the strict hierarchical pore structure it is the key factor to know both the transport and texture characteristics typical of its pore network. Pore structure depends not only on chemical composition, but also on the preparation method and has, therefore, to be determined experimentally. Experimental setups based on the inverse gas chromatography method (the Single Pellet String Column arrangement of the chromatography column) together with Graham's diffusion cell apparatus are utilized for the obtaining transport characteristics of tested ordered materials.

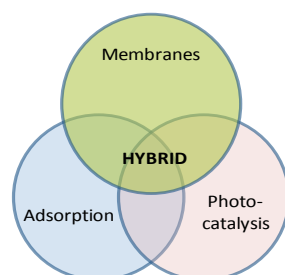


SEM micrographs of ZSM-5 zeolite coated on β -SiC foam (A, B, C and D)

Hybride membrane process for water treatment (HYMEPRO)

(O. Šolcová, L. Matějová (member of the steering group), solcova@icpf.cas.cz, 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. 23-25, 31, 32]



Production of 3rd generation biofuels by enzymatic catalyzed transesterification of microalgal oil

(O. Šolcová, solcova@icpf.cas.cz; joint project with EcoFuel Laboratories, s.r.o., 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 3rd generation of biodiesel production.



Scenedesmus obliquus

Biorefinery research centre of competence - BIORAF

(O. Šolcová, solcova@icpf.cas.cz; joint project with ICT, IBOT, Rabbit Trhový Štěpánov, a.s., Agra group, a.s., Briklis, s.r.o. and EcoFuel Laboratories, s.r.o.; supported by TACR, Competence Centres, project No. TE01020080)

The project employs the techniques of green chemistry for biomass utilization to the high added-value products and energy sources. By refining, it is possible to obtain food supplements, fodders and fertilizers, new-generation biofuels and energy from the biomass of microbial, plant or animal origin. Biorefining is a unique way of new sustainable substitution of fossil fuels minimizing the adverse effect on environment while exploiting the whole volume of biomass.

The project creates an interdisciplinary center with high innovation potential for sustainable utilization of renewable sources, and will bring the Czech Republic to the leading position in next-generation biorefinery within next eight years. The project links the private sector with experts from different fields of science (e.g., biosciences, phycology, analytical chemistry, enzymology, microbiology, chemical and biochemical engineering, material engineering, etc.).

Sustainable biomass resources, which will not compete with food crops in the use of agricultural land, will be employed in the project. New environmentally friendly processes for biomass biorefining will be developed in the order to obtain products with high market value and increase the market opportunities of participating companies, which will promote job creation. New technologies will be validated in the demonstration and pilot plant units; the developed products and technological processes will be commercialized.

Within four years, new intellectual property in the field of biorefinery will be created. The transfer of know-how from research to commercial sector will help to increase innovation potential and export opportunities of the participating companies. The project will bring the lend support to the Czech agriculture and industry and attract significant long-term investment opportunities in new technologies with high socio-economic impact.

Educational programs for graduates and young scientists have been developing to create experts in emerging technologies and opportunities for their employment. Finally, the project will contribute to the independence of the Czech Republic on fossil fuels and help to reduce the emissions of greenhouse gases.



Helinathus uberosus



Inulin syrup



Photo-bio-reactor



Crude microalgae oil

International co-operations

University of Ghent, Ghent, Belgium: Theory of chemical bond, theoretical characterization of aromaticity

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

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

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

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

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

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

University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix

Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Visualization of bonding interactions in transition metal complexes

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

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

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

University of Kragujevac, Serbia: Multicenter bonding, quantitative characterization of aromaticity

Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia: Morphology of PolyHIPE materials

University of Barcelona, Barcelona, Spain: Ion exchanger catalysts

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

University of Vigo, Vigo, Spain: Multicenter bonding, theoretical characterization of aromaticity
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
University of Liverpool, Liverpool, United Kingdom: Theory of chemical bond
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
Department of Physical chemistry, Slovak Technical University Bratislava, Slovakia: visualization of bonding interactions in transition metal complexes
Chemistry department, University of Pecs, Hungary: visualization of the bonding interactions in transition metal complexes
Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany: bonding in solids
Department of Chemistry, University of California-Davis, USA: electron reorganization in carbocationic rearrangements
Istanbul Technical University, Istanbul, Turkey: Synthesis and Thorough Characterization of Composite Functionalized Polymeric Nano-Structure

Visitors

L. Benoit, University of Strasbourg, France
M. Boltz, University of Strasbourg, France
D. Cooper, University of Liverpool, United Kingdom
B. Corain, University of Padua, Italy
J. Grabowski, Central Mining Institute, Katowice, Poland
M. Green, UCG Engineering Ltd, United Kingdom
P. Krajnc, University of Maribor, Slovenia
A. Lobnik, University of Maribor, Maribor, Slovenia
M. Pankiewicz, Central Mining Institute, Katowice, Poland
J. Rogut, Central Mining Institute, Katowice, Poland
A. Sezai Sarac, Istanbul Technical University Faculty of Sciences
A. Spojakina, Institute of Catalysis, BAS, Sofia, Bulgaria
K. Stanczyk, Central Mining Institute, Katowice, Poland
Y. Zub, Institute of Surface Chemistry NAS, Ukraine

Teaching

K. Jeřábek: visiting professor at Polymer Technology College, Slovenj Gradec, Slovenia, course "Functional polymers –morphology and application properties"
P. Klusoň: UJEP, course "Toxicology"
R. Ponec: CU, course "Structure and reactivity"
O. Šolcová: ICT, postgraduate course "Texture of porous solids"

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- [35] Krejčíková S., Kočí K., Obalová L., Čapek L., Šolcová O.: Chapter 24: Preparation and Characterization of TiO₂ - ZrO₂ Mixed Oxide Catalysts for Photocatalytic Reduction of Carbon Dioxide. In: *Chemistry for Sustainable Development*. (Gupta, B.M.- Jhaumeer-Laulloo, S. - Li, K.W., Ed.), pp. 389-398, Springer Science + Business Media B.V., Dordrecht 2012.

Patents

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