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Main 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 nanofibrous membranes and catalytic supports
- Assymetric Hydrogenations with Chiral Complexes in Ionic Liquids
- Advanced Hydrogen Storage Media

Applied research

- Catalytic combustion of volatile organic compounds
- Advanced oxidation processes for environment
- Textural characteristics of structural materials
- Green chemistry for biomass utilization to the high added-value products
- Enhancement of the power transformer operation security and failure prevention
- Decontamination of brownfields contaminated by organic compounds and heavy metals

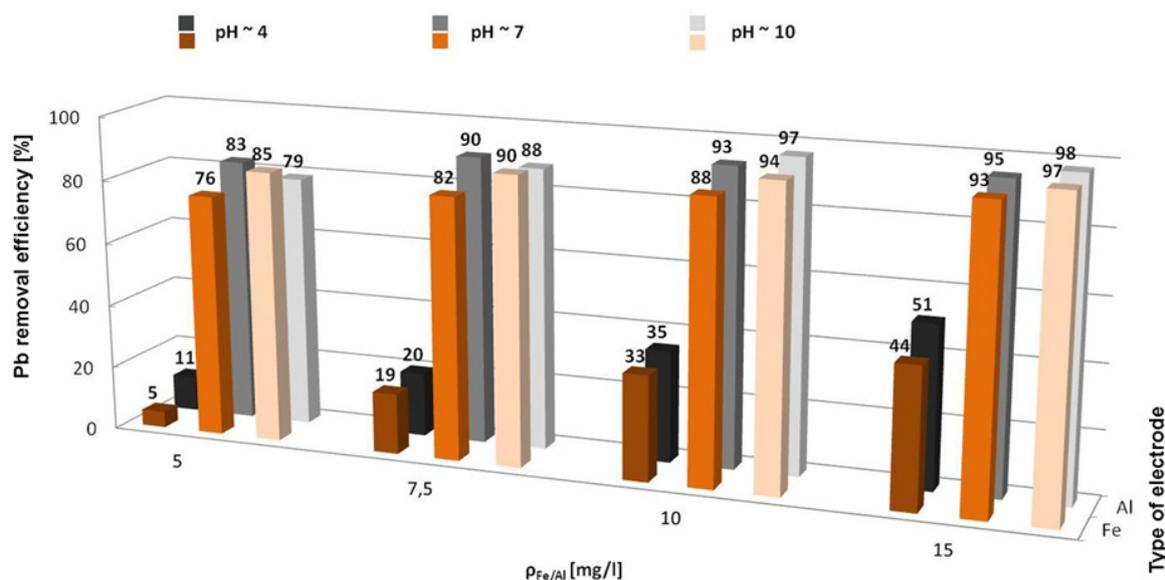
Research projects

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 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. 5]



Influence of initial pH on Pb removal efficiency

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

(L. Kaluža, kaluza@icpf.cas.cz; supported by European Union's 7th 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)

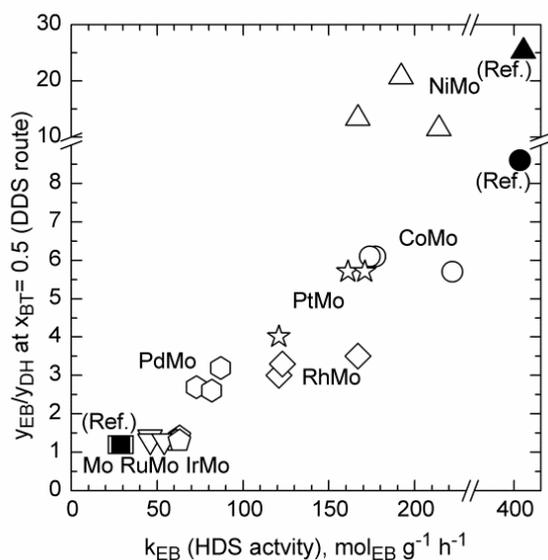
Catalysts were successfully prepared from five different experimental carbon blacks by impregnation with hexachloroplatinic acid, calcination, reduction and dechlorination. Calcination has been found to greatly increase the electrochemical stability. Dechlorination resulted in a 1.1–1.7-fold increase of the Pt crystallites, but did not alter the S_{BET} . Furthermore, the electroactive surface area (ESA) did not change significantly upon dechlorination, indicating that the purification and rearrangement taking place during the

dechlorination procedure are beneficial in terms of electrochemical utilization of the Pt. The prepared catalysts exhibited similar ESA of about $30 \text{ m}^2 \text{ g}_{\text{Pt}}^{-1}$, and all showed higher specific electrocatalytic activities toward the ORR than that of the commercial high-surface-area reference catalyst of $S_{\text{BET}} = 359 \text{ m}^2 \text{ g}^{-1}$, while their mass-specific ORR activities were slightly lower. All five catalysts showed better electrochemical stability of the support than the reference, which shows the benefit of using a support with moderate surface area. The stability of the Pt particles was better than the reference for one of the catalysts, namely Pt/CB3. This catalyst also had the highest S_{BET} ($193 \text{ m}^2 \text{ g}^{-1}$), the smallest Pt particles (6.1 nm), the best mass-specific ORR activity ($31 \text{ A g}_{\text{Pt}}^{-1}$) and the lowest residual Cl content (1380 ppm). It could be concluded that the high S_{BET} of CB3 within the moderate-surface-area CB supports is by far the most critical parameter influencing ESA and electrochemical stability. Catalyst manufacture based on the carbon type with large graphitic domains (CB5) was found to result in catalysts that perform poorly in terms of activities. [Refs. 12, 36]

Unconventional composition and preparation of sulfide hydrotreating catalysts

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

The 1-methyl-cyclohexene hydrogenation (o-HYD) was studied with 1-benzothiophene hydrodesulfurization (HDS) over Co, Ni, Mo, W, Rh, Re, Pd, Pt, Ir, CoMo, NiMo, RhMo, ReMo, PdMo, PtMo, IrMo supported catalysts. The CoMo/MgO catalysts exhibited at least 3.3-fold activities but the same selectivity C=C hydrogenation/C-S hydrogenolysis as the reference industrial CoMo/Al₂O₃ catalyst. Furthermore, mesoporous silica-aluminas (MSA) of different composition were studied as supports of Pd-Pt catalysts in transformation of refractory 4,6-dimethyldibenzothiophene (4,6-DMDBT). Activities of majority of Pd-Pt catalysts correlated with their Brønsted acidities. Pd-Pt/MSA catalysts were much more active than a conventional sulfide catalyst; the loadings around 0.10 wt. % gave 5-7 time more active catalysts than CoMo/Al₂O₃. [Refs. 10, 11, 30, 37]

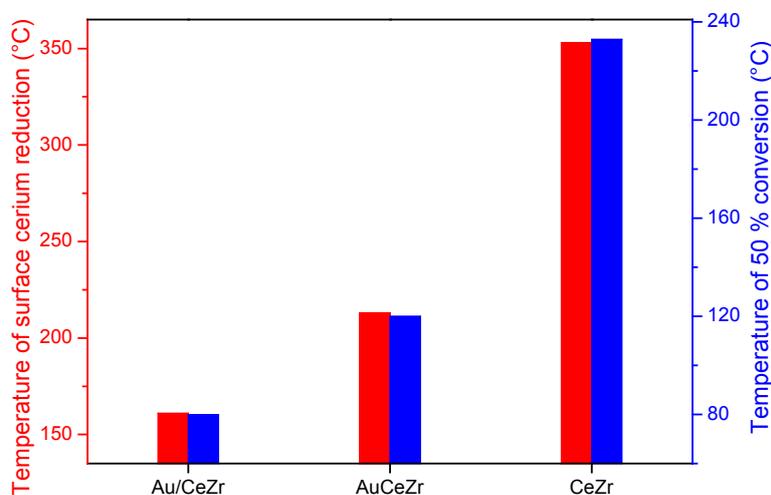


Correlation of relative selectivity direct desulfurization/hydrogenation desulfurization (DDS/HYD, $y_{\text{EB}}/y_{\text{DHBT}}$ at $x_{\text{BT}} = 0.5$) and overall HDS activity (k_{EB}) in hydrodesulfurization (HDS) of 1-benzothiophene over zirconia supported catalysts in laboratory tubular flow microreactor

Washcoated ceramic monoliths for total oxidation of volatile organic compounds

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

The innovative monolithic catalysts based on noble metals (platinum, palladium, gold) supported on electrospun nanofibre mats or on ceria-zirconia mixed oxide were studied. It was shown that except the type of noble metal, the key properties of the catalyst are noble metal loading and particle size, and that these properties depend on the method of catalyst preparation. By employing a proper preparation method, required physicochemical characteristics of the catalyst, especially reducibility and acidity, can be reached. Such catalysts then exhibit high activity and/or selectivity in the investigated reaction. However, it was also demonstrated that activity and selectivity of a given catalyst strongly depend on the type of volatile organic compound. Therefore, tailored synthesis of a catalyst is needed to achieve such combination of reducibility, acidity and resistance to poisoning, which would be suitable for a studied pollutant. The obtained results were published in impacted international journals. [Ref. 26]



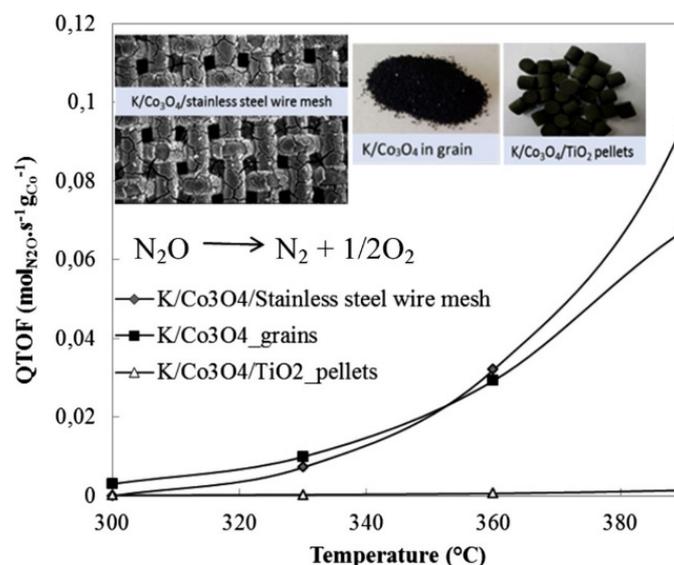
Correlation between reducibility of ceria-zirconia based catalysts and their performance in the elimination of model volatile organic compound (ethanol)

Structured catalysts with active oxide layer for removal of gaseous pollutants

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

Supported Co_3O_4 catalysts were prepared by heating of the cobalt hydroxide synthesized electrochemically on stainless steel sieves and by heating of the commercial TiO_2 pellets impregnated with cobalt nitrate solution. Mathematic simulation results showed that higher conversions in potential large scale application can be achieved over the catalyst deposited on stainless steel sieves in comparison with TiO_2 pellets. A significant increase in catalytic activity with increasing amount of cesium promoter was observed without respect to the Cs precursor.

Ethanol total oxidation over mixed oxide catalysts containing various transition metal cations was studied. The $\text{M}^{\text{II}}\text{-M}^{\text{III}}$ layered double hydroxide (LDH) precursors with $\text{M}^{\text{II}}/\text{M}^{\text{III}}$ molar ratio of 2 ($\text{M}^{\text{II}} = \text{Cu}, \text{Co}, \text{Ni}, \text{Cu-Ni}, \text{Cu-Co}, \text{and Co-Ni}$; $\text{M}^{\text{III}} = \text{Mn or Al}$) were prepared. The ternary mixed oxides containing Mn were more active than the binary Cu-Mn, Co-Mn, and Ni-Mn ones as well as the ternary Al-containing catalysts; the Cu-Co-Mn and Cu-Ni-Mn mixed oxides were the most active. The catalytic activity increased with increasing amount of easily reducible components and amount of oxygen desorbed from catalysts surface at lower temperatures (up to 500°C). [Refs. 8, 9, 15, 22, 37]



Influence of various catalysts on their efficiency

Assymmetric Hydrogenations with Chiral Complexes in Ionic Liquids - Reaction Engineering Aspects

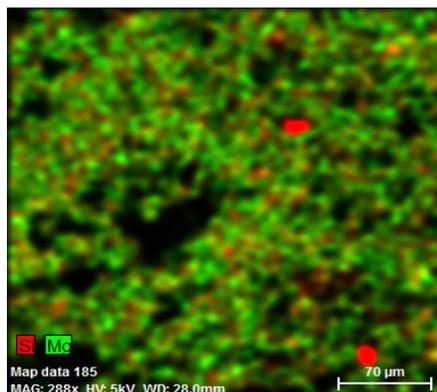
(P. Klusůň, kluson@icpf.cas.cz; supported by GACR, project No. 15-04790S)

In 2015 interactions of the catalytic Ru-BINAP complex with an inorganic matrix were studied and evaluated with help of XPS study. A detailed XPS study of interactions of [RuCl((*R*)-binap)(*p*-cymene)]Cl catalytic complex with Montmorillonite as characteristic type of inorganic support upon employing various types of immobilisation approaches was performed. This complex is typically used for stereoselective hydrogenations of β -ketosteres. It was shown that XPS is a method well suited for studying interactions of the Ru complex immobilised onto an inorganic matrix, either directly or via a heteropolyacid spacer. It informed on the surface stoichiometry, surface elemental composition, and energetic differences in the nearest vicinity of the main surveyed bonded elements. The interaction of Ru complex with an inorganic matrix via the heteropolyacid spacer is usually referred to as of covalent nature. Here it was shown that it was not at least clearly evident. The work could be understood as a model case study for many similar systems. The interaction of the catalytic Ru-BINAP complex with the model surface of Montmorillonite depends very much on the chosen method of immobilisation. The chemical form of the Ru complex plays also a certain role. Some effect of the used type of heteropolyacid was identified as well. For the Ru-BINAP complex either immobilised or in its standard crystal form there were no significant differences of the binding energies. On the other hand a shift towards higher E_B values for the dimer complex MDM was evident. For Ru-BINAP immobilised directly onto the Montmorillonite surface an increase of a binding energy appeared likely due to its interaction with an electronegative substituent. [Refs. 1, 2, 27, 31, 34]

Combined sorption modes for energy storage

(O. Šolcová, solcova@icpf.cas.cz; supported by GACR, project No. 15-14228S)

The project “Advanced Hydrogen Storage Media - Combined Sorption Modes” focuses on the design and preparation of high capacity sorbents for hydrogen storage via combination of chemisorption and physisorption processes. The first year of the project duration the major works within the task devoted to hydrogen storage assessment (based on determination of high-pressure adsorption isotherms of hydrogen and hydrolysis of silicides) were focused mainly on preparation and characterization of nanostructure materials (TiO₂, ZnO) including dopants based on sol-gel technique. [Refs. 3, 4, 6, 21]



Prepared magnesium silicides by EDX

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

(P. Klusoň, kluson@icpf.cas.cz; joint project with Teluria, TECHEM CZ; 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.



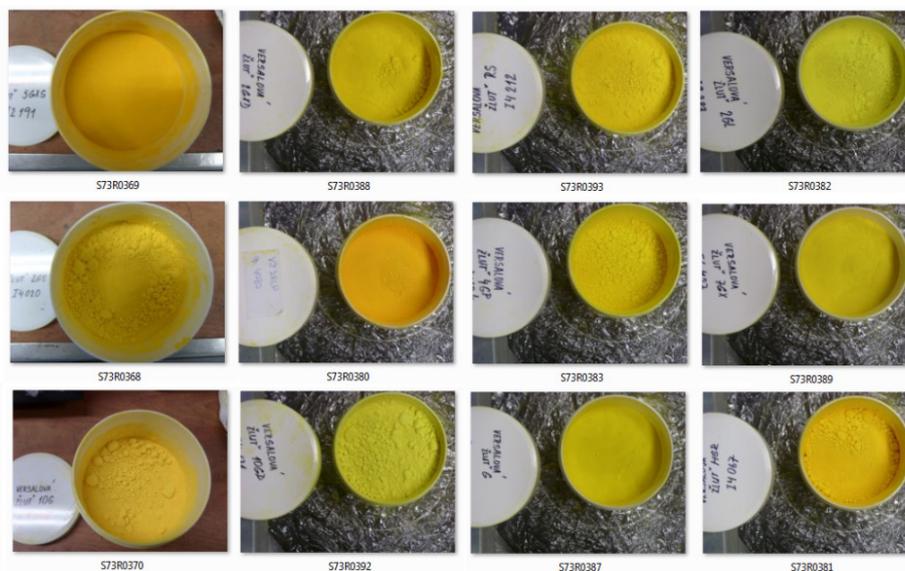
Emulsification progress with and without special additives

Ionic liquids as additives for special pigments

(O. Šolcová, 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. 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 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 ($N_{R,222}Tf_2N$, R = 6, 7, 8, 10, 12, 14) with a variable length of an alkyl chain are specially promising.



Differences of various pigment granulation

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; joint project with INVOS Ltd., COC Ltd., CU, ICPF, TU Brno; supported by TACR, project No. TA03010548)

In 2015 the detection system entitled Colour Clocks, and supported by the Technology Agency of the Czech Republic TACR, was successfully completed. Two types of light sensitive and precisely calibrated dosimeters were brought to the production level at the cooperation company Invos Ltd. The first dosimeter was denoted as the Gallery one. It is supposed to be used as part of strategies to protect valuable museum, archive and galleries artefacts. Light is generally known as one of the most critical factors to such items. It monitors the light exposure, and the recorded values could be than used to plan/limit future expositions, way of conservation, storage, transportation etc. Comparable systems are usually very expensive, based on sophisticated electronic devices, and requiring complicated technical equipment/support, and experienced operation, periodical control etc. The second system is denoted as the Derma-Clock, or as Derma dosimeter. Here, the target group is represented by standard users who seek of effective prevention when sunbathing. The high risk resulting from the exposure of the human skin to UV light from sun is generally known. It indicates, in the dependence of the skin sensitivity, the level of safe sun-light exposure, at different light conditions. It could be also corrected according to the applied sun protection factor of the used sunscreen cream. [Refs. 23, 24, 39, 40]

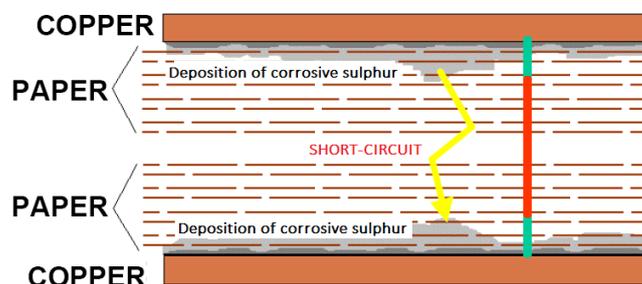


The first presentation of dosimeters to the public at the festival Night of Science, Brno, September 2015

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

(O. Šolcová, 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_2S , 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. [Refs. 14, 29]



Generating of short circuit

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

(F. Kaštanek, 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. [Ref. 17]



The newly designed mixotrophy reactor

Decontamination of brownfields extensively contaminated by organic compounds and heavy metals

(O. Šolcová, 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 separation 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 with. [Refs. 13, 19, 20, 25, 28]



Stainless steel laboratory thermal desorption apparatus

Electrochemical removal of toxic metals from polluted water

(P. Kluson, kluson@icpf.cas.cz; supported by TACR, project No. TA04020130)

The aim of the project “Electrochemical removal of toxic metals from polluted waters” is application of electrocoagulation method with following pilot scale testing on the treatment of industrially polluted waters. These waters contain dissolved metallic ions – especially ions of toxic elements ($\text{Cr}^{\text{III}+}$, $\text{Cr}^{\text{VI}+}$, $\text{As}^{\text{III}+}$, $\text{As}^{\text{V}+}$, $\text{Cu}^{\text{II}+}$, $\text{Cd}^{\text{II}+}$, $\text{Pb}^{\text{II}+}$, $\text{Co}^{\text{II}+}$, $\text{Ni}^{\text{II}+}$, $\text{V}^{\text{III}+}$, $\text{V}^{\text{V}+}$, $\text{Zn}^{\text{II}+}$, $\text{Al}^{\text{III}+}$). The attention will also be paid to removal of other noble metallic ions (e.g. Eu, Gd, Y, Yb) coming from electro-technical industry (compact fluorescent lamps, LCD panels, diodes, photovoltaic panels etc.).

The electrocoagulation technology has a great potential especially for treatment of specific waters coming from electro-technical industry with low concentrations of noble lanthanide and actinide group metals that can be after separation process returned back to the production process. That enables not only the industrial production frugality but also the production cost savings in consideration of price of these metals. Another broad area of application can be found in wastewater treatment coming from chemical, metallurgical, engineering or printing industrial sector. [Refs. 16, 18, 35, 38]



Electrocoagulation set-up

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 CAS)

Al₂O₃-CeO₂ supports containing 1-10 wt% Ce were prepared mechanochemically by milling aluminum and/or cerium nitrates with NH₄HCO₃. Heteropolymolybdate, (NH₄)₄NiMo₆O₂₄, was used as the precursor of the Ni and Mo to prepare NiMo₆/Al₂O₃-CeO₂ components in catalysts by impregnation method. The physicochemical properties of the catalysts were determined using chemical analysis, X-ray diffraction, temperature-programmed H₂ reduction, temperature-programmed NH₃ desorption, X-ray photoelectron spectroscopy (XPS), and the Brunauer-Emmett-Teller method. The catalyst acidity decreased with increasing Ce concentration in the support. XPS showed that the NiS/MoS ratio decreased two-fold for the Ce-modified alumina support. NiMo₆/Al₂O₃, which had the highest acidity, showed the highest activity in hydrodesulfurization of 1-benzothiophene (normalized per weight of catalyst). The concentration of surface MoO_xS_y species (which is equal to the concentration of Mo⁵⁺) gradually decreased to zero for catalysts with Ce concentrations higher or equal to 10 wt. %. However, the activities of all the catalysts prepared mechanochemically from Al₂O₃ and Al₂O₃-CeO₂ supports significantly exceeded that of a reference NiMo₆/Al₂O₃ catalyst prepared by impregnation method using the same precursor and with the same composition.

International co-operations

National University of Engineering, Lima, Peru: Determination of transport properties of the adobe brick building materials

University of Tumbes, Peru: Preparation and utilization of activated carbons prepared from agro-forestry biomass waste materials

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 and Hybrid membrane processes 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

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

University of Maribor, Maribor, Slovenia: PolyHYPE polymers

University of Barcelona, Barcelona, Spain: Ion exchanger catalysts

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

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

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

Publications

Original papers

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