UNIVERZITA J. E. PURKYNĚ V ÚSTÍ NAD LABEM
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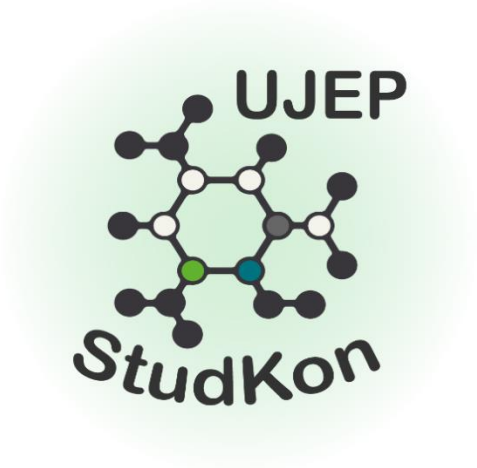
UNIVERZITA J. E. PURKYNĚ V ÚSTÍ NAD LABEM
Přírodovědecká fakulta



KNIHA ABSTRAKTŮ

Konference studentů přírodovědných a technických oborů UJEP

StudKon 2019

10. 6. – 11. 6. 2019
Dvůr Perlová voda, Budyně nad Ohří

http://www.studkon.ujep.cz

PROGRAM KONFERENCE

PONDĚLÍ 10. 6. 2019	
Registrace	8:00 – 9:00
Dopolední program	9:20 – 14:00
9:20 – 9:30	Zahájení a přivítání účastníků
9:30 – 10:50	Přednáškový blok 1
10:50 – 11:10	Coffee break
11:10 – 12:30	Přednáškový blok 2
12:30 – 14:00	Polední přestávka – oběd, krátký výlet, instalace posterů
13:00 – 14:00	Jednání oborové rady
Odpolední program	14:00 – 19:00
14:00 – 15:00	Přednáškový blok 3
15:00 – 15:20	Coffee break
15:20 – 16:00	Krátké představení posterů
16:30 – 18:00	Posterová sekce
18:00 – 19:00	Technická přestávka
Večerní program	19:00 – 22:00
19:00 – 19:30	Vyhlášení soutěže o nejlepší poster, vystoupení rektora univerzity a hostů
19:30	Večeře / raut
20:00 – 21:00	Kulturní společenský program – Kulatý stůl

ÚTERÝ 11. 6. 2019	
Dopolední program	8:30 – 12:30
8:30 – 9:30	Debata „Jsem Ph.D. a co dál“
9:30 – 9:50	Coffee break
9:50 – 11:30	Přednáškový blok 4
11:30 – 12:00	Technická přestávka
12:00 – 12:20	Vyhlášení soutěže o nejlepší přednášku, ukončení konference
14:00	Odjezd

SEZNAM PŘEDNÁŠEK A POSTERŮ

Přednáškový blok 1

- Eliška Wildová: Accumulation and dynamics of manganese content in plant species of forest ecosystem
- Michal Hošek: Disconcerting mercury hot spot and the Skalka Dam Reservoir as a mercury trap
- Jiří Štojdl: 10 tons of mercury in Skalka Dam Reservoir
- Jitka Tolaszová: Organic pollutants in sediments

Přednáškový blok 2

- Lukáš Bystrianský: Comparison of three quantification methods of microbial biofilm on polypropylene fibers
- Simona Lupínková: Sulphur microparticles grafted on UV-treated PET surface
- Martin Kozakovič: Granular vertical bladed mixer: flow patterns and homogenization
- Jiří Smejkal: Powder blasted glass microsystems for immunocapture of CTC

Přednáškový blok 3

- Martin Šťastný: Synthesis of blue luminescence metal diboride-based quantum dots by ultrasonication-assisted exfoliation
- Monika Benkocká: Functional nanostructured surfaces of polymer substrates for bioapplications
- Petr Ryšánek: Application of polymer nanofibers as antibacterial filtration media

Přednáškový blok 4

- Regina Herma: The new types of carbosilane dendrimers as non-viral transfection vectors for siRNA cell delivery
- Zuzana Nejedlá: Xenografts in Zebrafish and Dendrimers as Drug Delivery System
- Dominik Pilnaj: Application of drones for monitoring the troposphere quality
- Zdeňka Kwoczynski: Bioavailability of elements in lingo-cellulose matrix
- Hana Burdová: First results of Miscanthus x giganteus root exudates analysis

Postery

- Petr Aubrecht: Powderblasting and 3D printing technologies usable in fabrication of microsystems for immuno-capture of CTC
- Jan Dočkal: A general hydrogen bonding definition based on three-dimensional spatial distribution functions and its extension to quantitative structural analysis of solutions and general intermolecular bonds
- Jakub Ederer: Selected classical and instrumental analytical methods for the nanomaterials characterization
- Klára Jirounková: Surface Treatment of Al Alloy by PTA of HSS30 Steel
- Pavel Kraus: Grooved Shaft Analysis
- Diana Nebeská: Microbial and plant stress response during growing Miscanthus x giganteus in marginal lands: summary of first experiments
- Jakub Perner: Plasma modification of poppy seeds in fluidized bed reactor
- Eliška Rezlerová: Methane and Carbon Dioxide in Dual-Porosity Organic Matters: Adsorption and Diffusion as seen from Molecular Simulations
- Martin Smaha: Multi-dimensional gas chromatography coupled with mass spectrometry (GC x GC-MS) for circular economy and environmental applications
- Jiří Škvára: Molecular dynamics study of racemic mixtures: Temperature dependence of separation of ibuprofen racemic mixture with β-cyclodextrin in methanol solvent
- Jakub Tolasz: The influence of the preparation method of cerium oxide nanoparticles on its properties
- Štěpánka Tůmová: Comparison of stream and floodplain sediments for identification of individual sources of pollution in fluvial system (Panenský Creek, Czech Republic)
- Zuzana Žmudová: 3D Spheroids for Personalized Approach in Cancer Therapy

PŘEDNÁŠKY

Accumulation and dynamics of manganese content in plant species of forest ecosystem

*Eliška Wildová[a], Emanuel Kula[b]

[a] *Faculty of Environment, J. E. Purkyne University in Ústí nad Labem, Králova výšina 7, Ústí nad Labem, 40096, Czech Republic*

[b] *Faculty of Forestry and Wood Technology, Mendel University in Brno, Zemědělská 3, 61300, Brno, Czech Republic*

**presenting author, e-mail: wildova.eliska@gmail.com, 4th year of study*

Manganese is an essential element that belongs to the group of transition metals, and whose deficiency and excess in plants is manifested by chlorosis of assimilation organs [1]. The contribution deals with the level of Mn in assimilation organs of selected plant species growing on a permanent research area high on manganese in the soil (Ore Mountains, S: 50 ° 37 '03, 80''; V: 13 ° 37' 25, 17 "). Based on a long-term survey (2010–2018), the dynamics of Mn accumulation was defined for selected forest plant species (Bilberry - *Vaccinium myrtillus L.*, European Larch - *Larix decidua Mill.*, Silver Birch - *Betula pendula Roth*.) during the growing season (May–October). All of them showed increasing tendencies of Mn in leaves during the growing season with maximum values exceeding 10 000 $mg.kg^{-1}$. Blueberry was confirmed as a Mnaganese hyper-accumulator [2] that can tolerate high levels of Mn without showing any symptoms of manganese toxicity [3]. The influence of soil moisture and accumulated precipitation on increasing Mn content in bilberry leaves during the growing season was statistically proven. Monitoring of Mn in eastern Ore Mountains in bilberry leaves and its subsequent evaluation by geostatistical analysis proved the area of Litvínov to be very rich in Mn. The determined Mn content in soil (2016) did not correlate with the Mn content in bilberry leaves, but showed extremely elevated levels of Mn in soil in the area of interest. Nevertheless, the manganese contained in the soil is considered to be the main source of manganese in the plants, so the collected soil samples were measured by a portable XRF spectrometer. This method was effective for a quick determination of other elements in the humus and mineral horizons especially in an open terrain. To determine the reliability and accuracy of the portable X-ray spectrometry, the method was compared with the results from ICP-OES analysis and a significant correlation with the high determination index was demonstrated.

Research highlights

1) Long term research of Mn dynamics and accumulation in forest plant species
2) Dependence of Mn in bilberry leaves on soil moisture and cumulative rainfall
3) Monitoring of manganese in soil and bilberry leaves in eastern Ore Mountains
4) Comparison of two analytical methods (portable XRF vs. ICP-OES)

References

[1] PAVLOVÁ, Libuše. 2005: Fyziologie rostlin. 1st edition. Karolinum, Charles University in Prague, 382 p. ISBN 80-246-0985-1.

[2] KORCAK, R.F. 1989: Variation in nutrient requirements of Blueberries and other Calcifuges. Hort Science 24, 578 p.

[3]MILLER, P.M. 1987: Physiological responses of *Vaccinium vitis-idaea* to high tissue concentrations of manganese. J. Bot., 65: 1643–1646.

Disconcerting mercury hot spot and the Skalka Dam Reservoir as a mercury trap

*M. Hošek[a,b], T. Matys Grygar[a,b], , J. Popelka[a], J. Elznicová[a], Š. Tůmová[a], J. Bednárek[c]

[a] *Faculty of Environment, J. E. Purkyně University in Ústí nad Labem, Czech Republic*
[b] *Institute of Inorganic Chemistry, Academy of Sciences of Czech Republic, v.v.i., Řež, Czech Republic*
[c] *Povodí Ohře, state enterprise, Teplice, Czech Republic*
**presenting author, e-mail: hosek@iic.cas.cz (4th year of study)*

A key topic of current environmental geochemistry is legacy contamination, typically from mining. Surprisingly even today a "new" contaminated areas are being recognised even in Central Europe, such as mercury (Hg) hotspot downstream the Chemical Factory Marktredwitz (CFM;1788-1985) in east Bavaria, which produced Hg and its compounds, such as C_6H_5HgCl. This factory has harmed aquatic biota in the Kössein-Röslau-Ohře river system. Although the factory is out of service for over 30 years, total Hg concentration in floodplain sediments is in order x00 mg/kg, while an Earth crustal average is 0.05 mg Hg/kg and environmental safety limit in soils is ca. 1.5 mg/kg. Because suspended particulate matter (SPM) is one of the most important transport medium of pollutants in the aquatic environment, I constructed SPM samplers resembling Phillips tubes, and placed them both in the contaminated river system and the Ohře River above to confluence with the Röslau River, as an unpolluted point. We also used datasets from monitoring of the Ohře River by Povodí Ohře. The Röslau River currently export SPM with mean Hg concentrations ca. 20 mg/kg Hg, transported by the river system to the Skalka Dam Reservoir.

Two kinds of Hg pollution hotspots can be found in developed countries: Hg mining sites, such as downstream the Almadén Area, Italy (the world's 3rd largest Hg mine) and chemical factories, such as Babeni Reservoir in the Olt River, Romania (the largest chlor-alkali plant in Central and Eastern Europe). Mining has usually produced more Hg waste in terms of amount, while chemical factories has produced more bioavailable Hg [1]; the CFM is in between those end-members, i.e., it is comparably serious. Mercury is bioaccumulated in aquatic biota of the upper Ohře River persistently. Fish in the Skalka Dam Reservoir have had Hg concentrations in their muscles of up to 6 mg/kg, many times exceeding the hygienic limit (0.5 mg/kg). According to literature [2], 1 mg/kg Hg in adult fish cause 24% injury, while 5 mg/kg Hg cause 78% injury. Based on floodplain drill cores we deciphered, that most of contamination is concentrated primarily in channel belt. The Hg inventory in the Kössein-Röslau river stretches was therefore estimated from typical width of the channel belt, mean Hg concentrations, and thickness of the polluted strata. It produced estimate of ca. 13 t Hg in a 22 km long channel belt, which is prone to fluvial remobilization during floods. Although a major portion of the fluvially transported Hg has yet been trapped by the Skalka Reservoir, the SPM exported farther downstream still varies between 2 and 10 mg/kg Hg depending on the river discharge. Although revitalization should be a necessity, it must be done sensitively and after assessing the palpable risk of mercury remobilization.

Research highlights

1) 13 t Hg is dispersed in a 22 km long channel belt of the Kössein-Röslau river system
2) SPM brought to Ohře River and Skalka Dam Reservoir ca. 20 mg/kg Hg
3) Fish in the Skalka Dam Reservoir with Hg concentrations in muscles of up to 6 mg/kg

References:

[1] A.G. Bravo, C. Cosio, D. Amourou, J. Zopfi, P.A. Chevalley. Extremely elevated methyl mercury levels in water, sediment and organisms in a Romanian reservoir. Water Res. 49, (2014), 391–405.

[2] T. Dillon, N. Beckvar, J. Kern. Residue-based Mercury Dose-response in Fish. Environ. Toxicol. Chem., 29, (2010), 2559–2565.

10 tons of mercury in Skalka Dam Reservoir

*Jiří Štojdl[a], Jitka Elznicová[a], Tomáš Matys Grygar[a,b,] Ondřej Bábek[c], Zuzana Lenďáková[c]

[a] *Faculty of Environment, J.E. Purkyně University in Ústi nad Labem, Czech Republic*
[b] *Institute of Inorganic Chemistry AS CR, v.v.i., Řež, Czech Republic*
[c] *Department of Geology, Palacký University Olomouc, Czech Republic*

**presenting author, e-mail: Jiri.stojdl@ujep.cz, 3rd year*

Dam reservoir sediments are used as archives of contamination, eutrophication and soil erosion in their catchment area. Numerous recent research reports on reservoir sediments have been based on a random sampling of single or a few sediment cores without prior knowledge on the bottom bathymetry and reservoir deposition patterns. Such an approach can produce misleading results because the deposition in the reservoir bottom is in fact quite uneven and the finest bottom sediment is being reworked by waves, currents and water level manipulations.

We will show an example of using bathymetry in the research of contamination in the bottom sediments of the Skalka Dam Reservoir, the Czech Republic, situated near the Czech-German border. The Skalka Reservoir has received Hg contamination [1] from a historical chemical factory in Marktredwitz, Germany [2]. We started our research by collecting data on the reservoir depth to construct the bathymetry map. We used ordinary fish-finder sonar (Humminbird Helix) attached to an inflatable boat with an electric motor. We also performed ground penetrating radar (GPR) measurement in the reservoir inflow, which visualised sub-bottom layers interpreted as pre-dam structures or events such as single extreme floods. The results of sonar imaging and GPR measurement were compared with historical maps of the pre-dam channel position. Sampling points were then selected to cover each sedimentary body in the bottom: depressions in the pre-dam channels, abandoned channels, reservoir basin in the pre-dam floodplain and valley slopes. Because Hg determination is time-consuming, we used Zn concentration of a proxy for Hg content, as both Hg and Zn were jointly in the effluents from the Marktredwitz factory [2,3]. The Zn concentration was available by plain XRF analysis.

We distinguished 4 sedimentary areas with distinct depth profiles of Hg and Al/Si and Zr/Rb ratios for calculating total Hg content. Based bathymetry with GPR and core data was calculated the amount of sediment for each area and then calculated the approximate content of mercury in sediment. The sum of all areas is 10 tons of mercury in 1 100 tons of sediment.

Research highlights

1) Combined bathymetry, GPR and core sampling to identify of pre-dam bottom
2) Using of Zn concentration as a proxy for Hg content
3) Identification of four reservoir deposition areas for calculation of Hg amount
4) In sum ca. 10 tons of Hg has been deposited in Skalka Dam Reservoir

References

[1] Majerová, L.et al. Dam reservoirs as an efficient trap for historical pollution: the passage of Hg and Pb through the Ohře River, Czech Republic. Environ. Earth Sci. 77 (2018) 574.
[2] Selim, H. M., Iskandar, I. K. Fate and transport of heavy metals in the vadose zone. Boca Raton, Fla.: Lewis Publishers, 1999, pp. 300 and further. ISBN 0-8493-4112-4.
[3] Matys Grygar, T., Elznicová, J., Kiss, T., Smith, H. G. Using sedimentary archives to reconstruct pollution history and sediment provenance: The Ohře River, Czech Republic. Catena 144, 109–129 (2016).

Organic pollutants in sediments

*Jitka Tolaszová[a], Sylvie Kříženecká[a], Jitka Elznicová[a] and Tomáš Matys Grygar[a,b]

[a] *Faculty of Environment, Jan Evangelista Purkyně University in Ústí nad Labem, Králova Výšina 3132/7, 400 96 Ústí nad Labem, Czech Republic*
[b]*Institute of Inorganic Chemistry AS CR, v.v.i., 25068 Řež, Czech Republic*

**Jitka Tolaszová, e-mail: jitka.tolaszova@ujep.cz*

Sediments provide valuable geochemical records of the past local and regional changes of the past environment. River floodplains and dam reservoirs are particularly suitable for that purpose. The selection of sampling points in floodplains must start by examination of historical and current maps and aerial photographs. Other useful information provided by sediment analysis is the historical development of anthropogenic influences in the basin over the last centuries. To determine the age of sediments, it is possible to use information from geoinformation systems on the movements of the river bed in the past, provided that we are interested in events that are captured on maps, aerial photographs, drawings of the trough belt and similar archive information. From an environmental point of view, especially highly polluted sediments are being studied nowadays due to their acute toxicity. The basic approach to assessing sediment contamination, which is also the approach required by legislation, is to compare the found concentrations of pollutants with tabulated values of the maximum permissible values for a certain type of matrix, such as sediment, soil or water. Organic pollutants are ubiquitous in the sediments. The problem is that for many of the currently used organic pollutants (pesticides) there are no legislative limits in sediment pollution in the Czech Republic. It may be related to the fact that for numerous pollutants there are no established and validated analytical procedures (extraction from solid matrix and determination) and reference materials. This is due to the lack of legislation, but also to a very small number of publications concerning organic pollutants in real sediments. Analytical methods developed so far have focused on selected nonpolar analytes with a high Koc distribution coefficient and therefore a high affinity for sediments. Here a lot of fundamental analytical research is still required, in particular polar pesticides, introduced late in 20th century to replace non-polar pesticides. Unfortunately, some polar pesticides have already been revealed as persistent and dangerous.

To assess the contamination by organic pollutants, the sediments were sampled, homogenized, extracted and analyzed. For the isolation of organic pollutants from sediment matrix, a mechanical disrupter MiniG™1600 was used. Due to the large number of samples, a fast extraction procedure with the minimum amount of a used sample and solvents for the determination of organic pollutants has been developed. For the analysis of organic pollutants, a 7890B gas chromatograph with a 7000D triple quadrupole mass spectrometer and a 1290 Infitity II liquid chromatograph with a 6495 triple quadrupole mass spectrometer were used. A universal validated analytical method that would be widely used in accredited laboratories for the determination of large quantities of analytes of different chemical groups in sediments is missing. We would like to partially fill that gap.

Research highlights

1) Analysis of large quantities of analytes of different chemical groups in sediments.
2) Reproducible extraction techniques.
3) Use of a small amount of a sample as well as a solvent for the extraction.

Comparison of three quantification methods of microbial biofilm on polypropylene fibers

Lukáš Bystrianský[1], Milan Gryndler[1] and Martina Hujslová[2]

[1]Faculty of Science, Department of Biology, J. E. Purkyně University in Ústí nad Labem, České mládeže 8, CZ40096, Ústí nad Labem, Czech Republic

[2]Laboratory of Fungal Biology, Institute of Microbiology ASCR, v.v.i., Vídeňská 1083, CZ14220, Prague 4, Czech Republic

**Lukáš Bystrianský, 4. ročník, e-mail: m.leafs@seznam.cz*

The biofilms represent living forms of microorganisms (bacteria, fungi, algae, protozoa) which are adhered by self-produced extracellular matrix to the biotic or abiotic surfaces [1]. They are ubiquitous in nature and represent important biological entities. For some studies of biofilms, it is necessary to evaluate their quantity. Some quantification methods have been established for biofilms but a universally applicable one is missing. Each method has its own limitations that may distort the results and the choice of a suitable method may be a challenging task [2]. The most frequent are staining methods using cell dyes (crystal violet, safranin) or fluorogenic DNA dyes (ethidium bromide, PicoGreen, Syto9) [3].

In our experiment, we proposed a quantification method based on measuring of oxidizable organic carbon in biofilm biomass (based on bichromate oxidation) [4]. We compared the results obtained using this method with results of 2 other commonly used method (crystal violet destaining and measuring of extracted DNA concentration). We cultivated the microbial biofilm on the surface of polypropylene fibers in a nutrient medium inoculated by suspension of two different soils. We investigated the effect of salt concentration and valence on the amount of the produced biofilm and composition of biofilm microbial communities.

The bichromate oxidation is a simple and fast method and our results showed that it is more sensitive than crystal violet destaining. Moreover, the bichromate oxidation method provides lower background. DNA staining, especially by PicoGreen, is sensitive but, on the other hand, may be time-consuming and relatively expensive.

The sequencing revealed, that biofilm bacterial communities developed from both soils were very different but the effect of salt valence was statistically significant ($p \leq 0.05$) only in some OTUs (*Arthrobacter*/*Peudarthrobacter*/*Paenarthrobacter* and *Bacillus* with positive response to KCl as monovalent salt and *Streptomyces*, *Lysinibacillus*, *Pseudomonas* and *Ensifer* with positive response to $MgSO_4$ as bivalent salt). The significant preference for a certain concentration of salts was observed in the case of OTUs *Agrobacterium* (100mM) and *Bacillus* (100mM) from Soběnice soil and *Brevundimonas* (30mM) from Soos soil.

Research highlights

1) Bichromate oxidation as a new quantification method of biofilm biomass.
2) The assessment of salt concentration and valence on the amount of produced biofilm and composition of biofilm communities.

References

[1] M. E. Davey, G. A. O´Toole. MaMBR, 64, (2000), 847.

[2] I. Randrianjatovo, E. Girbal-Neuhauser, C. E. Marcato-Romain. AMaB, 99, (2015), 4835-4844.

[3] S. Stepanovic, D. Vukovic, I. Dakic, B. Savic, M. Svabic-Vlahovic. JoMM, 40, (2000), 175-179.

[4] J. R. Sims, V. A. Haby. Soil Science, 112, (1971), 137.

Sulphur microparticles grafted on UV-treated PET surface

*S. Lupínková[a], K. Kolářová[b], P. Sajdl[b], Z. Kolská[a]

[a]*Materials Centre of Ústí nad Labem and Department of Physics, Faculty of Science, J. E. Purkyně University, Ústí nad Labem, Czech Republic*
[b]*Department of Solid State Engineering, Faculty of Chemical Technology, University of Chemistry and Technology, Prague, Czech Republic*
**presenting author, e-mail: simona.lupinkova@email.cz*

Sulphur is a widely used element in different applications such as fertilizers, pharmaceuticals, antimicrobial agents, insecticides and fumigants. Sulphur nano- and microparticles are nowadays useful for modification of metal and carbonnanotubes, synthesis of composites for lithium batteries, anti-cancer agent, antibacterial agentand as adsorbent for the extraction of metal ions [1,2].

In this work, we have studied the surface properties of polyethylene terephthalate (PET) foil and changes in its surface properties after activation by ultraviolet radiation and subsequent grafting with sulphur microparticles (SMPs). SMPs have been prepared by an acid catalysed precipitation of sodiumthiosulphate in the presence of Tween 20, PEG-400 or chitosan as a stabilizers and size-control agents.

The surface wettability was determined by goniometry from static contact angle measurement. Surface chemistry and surface charge were studied by electrokinetic analysis. Changes in surface chemical structure were characterized by X-ray photoelectron spectroscopy (XPS). Selected samples were tested for antimicrobial activity.

Research highlights

1) Efficient UV activation of PET surface for subsequent grafting
2) Preparation of sulphur microparticles with narrow size distribution
3) Efficient grafting of sulphur microparticles on PET surface
4) Changes in surface properties demonstrated by used analytical methods

Acknowledgement

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References

[1] R.G. Chaudhuri, S. Paria. J. Colloid Interface Sci. 343, 2, (2010), 439.
[2] X. Xie, R. Deng, Y. Pang, Y. Bai, W. Zheng, Y. Zhou. Chem Eng J. 314, (2017), 434.

Granular vertical bladed mixer: flow patterns and homogenization

*Martin Kozakovic[a], Jaromir Havlica[a, b]

[a] *Faculty of Science, UJEP, České mládeže 8, 400 96 Usti nad Labem, Czech Republic*

[b] *ICPF Czech Academy of Sciences, Rozvojová 2/135, 165 02 Prague, Czech Republic*

**presenting author, e-mail: martin.kozakovic@gmail.com, 1 year of PhD. degree*

This contribution is focused on the mixing of the dry granular material in a vertical cylindrical mixer with two opposed flat blades with a 45° rake angle. The computational simulation of the mixing was performed for 42212 monodisperse spherical glass particles. The problem of the homogenization process has been solved by many scientists since 1950s, but there is still resistance to understand the complex behavior of granular flow. Our motivation was to interpret the complex behavior of the granular flow by using computational techniques. We tried to describe the connection between dynamics of primary and secondary granular flows and the homogenization process during the convection mixing mechanism. Fig. 1 presents an evolution of concentration fields for blades rotational speed 150 rpm and two different initial packing configurations (tangential and radial). For a tangential initial configuration (Fig 1a), it is possible to monitor the effect of primary flows (tangential velocity) on the homogenization process. On the other hand, Fig 1b illustrates the importance of secondary flows for mixing process especially for initial packing configuration with phase interface oriented in the tangential direction to the primary flow. Based on these results, ideal working conditions were determined for investigated mixing process.

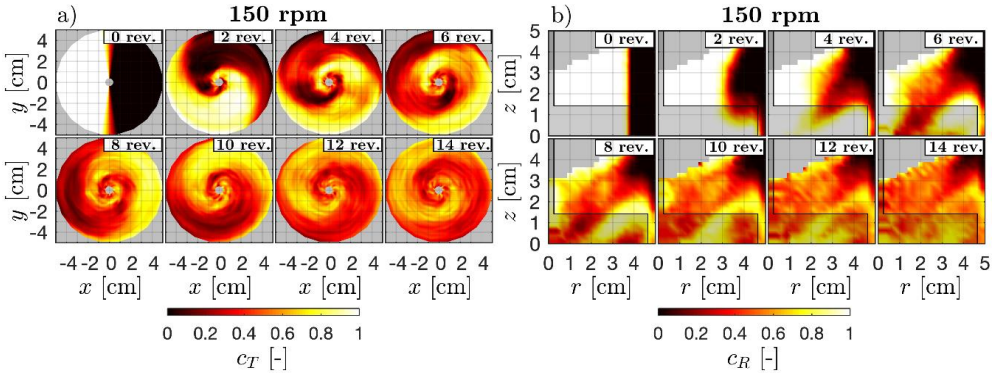

Figure 1. 2D concentration patterns for a) side-by-side and b) inside-outside initial packing. The stirrer is semi-transparent. The blades rotational speed is 150 rpm.

Research highlights

1) Transformation of 3D to 2D velocity fields detects the recirculation zones.
2) Recirculation zones support the process of homogenization.
3) Optimal working conditions were suggested for cylindrical mixer.

References

[1] J. Havlica, K. Jirounkova, T. Travnickova, M. Kohout, Powder Technol. 280 (2015), 180–190.
[2] T. Barczi, T. Travnickova, J. Havlica, M. Kohout, Chem. Eng. Technol. 38 (2015), 1195–1202
[3] J. Havlica, K. Jirounkova, T. Travnickova, P. Stanovsky, P. Petrus, M. Kohout, Powder Technol. 334 (2019), 79–88.

Powder blasted glass microsystems for immuno-capture of CTC

[*]Jiří Smejkal[1], Petr Aubrecht[1], Alena Semerádtová[1], Marcel Štofik[1] and Jan Malý[1]

[1]*J.E. Purkyně University, Faculty of Science, Ústí nad Labem, Czech Republic*
**presenting author, e-mail: jiri.smejkal@ujep.cz, 3rd year of Ph.D. training*

Development of microsystems for cell-based studies is very demanding in biomedical research and has many possible applications, capturing of circulating tumor cells (CTCs) cells in particular. A lot of recent development was done in the field of capturing CTCs using microsystems [1]. In addition to the very widespread microfabrication method of soft lithography, powder microblasting can be a microfabrication technology suitable for rapid prototyping and fast micromachining of microsystems [2] for cell-based studies. In our work, the powder blasted glass microsystems for receptor-based cell immobilization and shear stress testing are presented as the microsystems suitable for immuno-capture of rare CTCs.

The microsystems were fabricated by the powder microblasting technology. As substrate material for microfabrication, microscopy glass slides and common glassing panels were used. All fabricated parts were bonded together with the biocompatible transfer contact, which also served as the microfluidic channel.

On the substrates, different biotinylated antibodies (EpCam – specific antibody for cell capture, Anti-Mouse IgG – non-specific antibody) were immobilized. The sandwich of immobilized antibodies was built on silanized glass substrates using the (3-Aminopropyl)triethoxysilane, biotin-PEG-COOH, and streptavidin. MCF7 cell line (ATCC® HTB-22™ adenocarcinoma cell line) was used as the model CTCs for our tests, due to their ability to overexpress EpCam receptors on their surface.

Receptor-based cell immobilization and shear stress tests, were observed and documented by the inverted fluorescent microscope Olympus IX 71 coupled with the CCD camera. Data were acquired and evaluated by using appropriate software for automated microscope control, thus opening the possibility of parallelization and automated data processing was successfully accomplished.

The presented static and dynamic systems were cheap to fabricate, quick and easy to assemble. Due to their construction and design, receptor-based cell immobilization and shear stress testing on different substrates was optimized with the minimal volume of antibodies. Performed tests have shown, that model CTCs cell line can be successfully captured.

Research highlights

1) Fast and painless liquid biopsy analysis.
2) Minimal reagent consumption.
3) Quick analysis.
4) Cheap materials.

References

[1] SUN, Yuxi, Thomas A. HAGLUND, Aaron J. ROGERS, Asem F. GHANIM a Palaniappan SETHU. Review: Microfluidics technologies for blood-based cancer liquid biopsies. Analytica Chimica Acta [online]. 2018, 1012, 10–29. ISSN 00032670. doi:10.1016/j.aca.2017.12.050

[2] SOLIGNAC, D., A. SAYAH, S. CONSTANTIN, R. FREITAG a M. A. M. GIJS. Powder blasting for the realisation of microchips for bio-analytic applications. Sensors and Actuators A: Physical [online]. 2001, 92(1–3), Selected Papers for Eurosensors XIV, 388–393. ISSN 0924-4247. doi:10.1016/S0924-4247(01)00577-5

Synthesis of blue luminescence metal diboride-based quantum dots by ultrasonication-assisted exfoliation

*Martin Šťastný[a], Václav Štengl[a], Daniela Popelková[a] and Jiří Henych[a]

[a] *Institute of Inorganic Chemistry of the Czech Academy of Sciences, 25068, Řež, Czech Republic*

**presenting author, e-mail: stastny@iic.cas.cz*

The top-down exfoliation involves the exfoliation of a bulk layered material down to monolayer 2D nanosheets. Ultrasonication-assisted liquid-phase exfoliation has emerged as an efficient method for producing large quantities of 2D nanostructures such as graphene [1] and its analogs (molybdenite or wolframite) [2], as well as synthetic layered compounds (h-BN, h-BCN, g-C_3N_4) [3]. This work explores the use of ultrasonication-assisted exfoliation to produce a new class of boron-rich, layered quantum dots, namely metal diborides (TiB_2, MgB_2, MoB_2, HfB_2, and AlB_2) and investigate their properties using characterization methods (UV-Vis spectroscopy, HRTEM, XRD). Metal diborides (MB_2) are a class of structurally related materials that contain hexagonal sheets of boron separated by metal atoms with wide applications due to their extremely high melting points (> 2500 °C), high mechanical hardness, good electrical and thermal conductivity and chemical inertness [4]. Quantum dots are used in electronics such as single-photon detectors, lasers, optical memory, laser pointers, or in medicine for diagnosis and invasive therapy of all kinds [5]. Results not yet published show that ultrasonication-assisted liquid-phase exfoliation is an effective method for facilitating the production of 2D metal diboride-based quantum dots with the diverse application (e.g., for barrier protection against classical metal corrosion or UV corrosion of plastics).

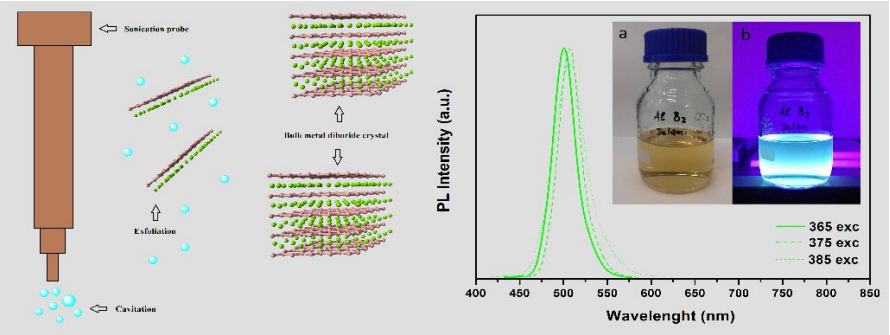

Figure 1 Schematic diagram showing ultrasonication-assisted exfoliation of metal diborides (left); PL spectra of the AlB_2 quantum dots: Sample seen under visible light (a) and under UV light (b).

Research highlights

1) A new method for synthesizing metal diboride-based quantum dots was used
2) Quantum dots suitable for barrier protection against metal corrosion or UV corrosion of plastics.

References

[1] V. Štengl. Chem. - A Eur. J. 18 (2012), 14047–14054.
[2] V. Štengl, J. Henych. Nanoscale. 5 (2013), 3387–3394.
[3] V. Štengl, J. Henych, M. Kormunda. Sci. Adv. Mater. 6 (2014), 1106–1116.
[4] W.G. Fahrenholtz, G.E. Hilmas, I.G. Talmy, J.A. Zaykoski. J. Am. Ceram. Soc. (2007).
[5] A. Valizadeh, H. Mikaeili, M. Samiei, S.M. Farkhani, N. Zarghami. Nanoscale Res. Lett. (2012).

Functional nanostructured surfaces of polymer substrates for bioapplications

*Benkocká Monika[a], Kolářová Kateřina[b], Herma Regina[a] and Kolská Zdeňka[a]

[a] *Faculty of Science, J. E. Purkyne University in Usti nad Labem, České mládeže 8, 400 96 Usti nad Labem, Czech Republic*
[b] *Department of Power Engineering, Institute of Chemical Technology in Prague, 166 28, Prague 6, Czech Republic*

**presenting author, monika.benkocka@ujep.cz; 4th year of PhD study*

Polymeric materials have recently been replacing traditional engineering materials with their great abilities, such as better corrosion resistance, lightness, flexibility, low cost. However, their surface properties, wettability, biocompatibility or adhesion may limit their further potential use. It is necessary to improve these surface properties using different physical (plasma) or chemical (Piranha solutions) methods. The purpose of this modification is to provide reactive sites on the surface to facilitate the binding of other selected compounds. These new substrates can be used for various medical purposes, bioapplications.[1-3]

Changes in the surface properties of the studied substrates were characterized by various analytical methods. The surface chemistry was determined by measuring the electrokinetic potential (zeta potential), to determine the elemental composition, X-ray photoelectron spectroscopy was used, wettability was determined by goniometric measurement of the contact angle. On modified surfaces, tests for antimicrobial activity have been performed. Also, tests for cell adhesion and proliferation have been carried out on nanostructured surfaces.

Research highlights

1) Successful chemically grafting changes surface chemistry, polarity and wettability
2) Modified surfaces exhibit antibacterial properties
3) Selected samples are even “cell-friendly” for cell adhesion and proliferation
4) New cheap and stable nanocomposites with antimicrobial properties for bioapplications

References

[1] Benkocká M., Kolářová K., Matoušek J., Semerádtová A., Šícha V., Kolská Z.: Nanocomposite of polystyrene foil grafted with metallaboranes for antimicrobial activity, Appl. Surf. Sci. 441, 120–129, 2018.

[2] Benkocká M., Lupínková S., Matoušek J., Kolářová K., Kolská Z.: Antibacterial and photophysical properties of chemically modified PET foil, RSC Advances 8, 15001 – 15008, 2018.

[3] Benkocká M., Lupínková S., Knapová T., Kolářová K., Matoušek J., Slepička P., Švorčík V., Kolská Z.: Antimicrobial and photophysical properties of chemically grafted ultra-high-molecular-weight polyethylene, Mater. Sci.& Eng. C 96, 479-486, 2019.

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Application of polymer nanofibers as antibacterial filtration media

*Ryšánek, P.[a], Čapková, P.[a], Štojdl, J.[b], Trögl, J.[b], Malý, M.[a], Kolská, Z.[a], Kormunda, M.[a], Benada, O.[b,c], Munzarová, M.[d]

[a]*Faculty of Science, J. E. Purkyně University, České mládeže 8, 400 96 Ústí nad Labem, Czech Republic*
[b]*Faculty of Environment, J. E. Purkyně University, Králova výšina 3132/7, 400 96 Ústí nad Labem, Czech Republic*
[c]*Institute of Microbiology of the Czech Academy of Sciences, Vídeňská 1083, 142 20 Prague 4, Czech Republic*
[d]*Nanovia, s. r. o., Litvínov, Podkrušnohorská 271, 436 03 Litvínov – Chudeřín, Czech Republic*
**presenting author, 3rd year, Ph.D. Applied Nanotechnologies e-mail: petr.rysanek@ujep.cz*

Nanofiltration with additional antibacterial effect is still one of the big challenges in applied nanotechnology. Due to bio-fouling have pure nanofilters lower durability and efficiency for filtration. The solution for this problem, are antibacterial filtration membranes, which are designed for high efficiency, because they have large antibacterial activity. The aim of this research is to investigate the best combination of polymer and modifying agent, and also to determine the stability of the prepared antibacterial membrane.

Antibacterial membranes were prepared by one-step synthesis using laboratory Nanospider technology. Two polymers and three modifying agents were tested. For the evaluation of the presence of the agents on the nanofiber surface the XPS, SEM, XRD and electrokinetical measurements were used. The experimental results were also compared with molecular modelling. All the membranes were also tested on their antibacterial effect.

The best combination of polymer and antibacterial agent was tested on special air-blowing device, to confirm the stability of the modification. The tests lasted for three weeks and the results validated very good stability of this complex, and also very good antibacterial activity after air-blowing testing. This fact is significant for future applications for example in air-conditioning devices.

Research highlights:

1. One-step synthesis of antibacterial nanofibers
2. Determination of changes in structure, morphology, surface chemistry
3. Testing of antibacterial activity
4. Observation antibacterial modification stability during air-blowing

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The new types of carbosilane dendrimers as non-viral transfection vectors for siRNA cell delivery

*Regina Herma[a], Dominika Wrobel[a], Michaela Liegertova[a], Monika Mullerova[a, b], Tomas Strasak[a,b], Marcel Stofik[a] and Jan Maly[a]

[a] *Faculty of Science, J.E. Purkyně University in Ústí nad Labem, 40096 Ústí nad Labem, Czech Republic*

[b] *Institute of Chemical Process Fundamentals of the CAS, v.v.i., Prague, Czech Republic*

**presenting author, fourth year of study, e-mail: hermaregina@gmail.com*

Rapidly developing concepts of gene therapy bring great expectations in potential treatment of several fatal genetic-based diseases as are cystic fibrosis, haemophilia, various types of neurodegenerative diseases, HIV infections and cancers.[1] The core of the approach lies in the specific local delivery of nucleic acids (DNA, small interfering RNA (siRNA)) in to the targeted cells to mediate the therapeutic effect on selected genes. Based on the type of nucleic acid, the genetic material must be transported either into the nucleus (DNA) or into the cytosol of the cells (siRNA). The indispensable part of the functional gene therapy concept is the availability of suitable nucleic acid carriers.

Dendrimers (DDMs) represent a group of nearly monodispersed, highly symmetric polymeric nanoparticles. Their near-spherical shape at higher so-called generations (G), small size (mostly 1-10nm), well controllable composition of their core and shell and wealth of surface modification strategies make from them potentionally successful candidates in gene delivery applications.

We have shown that in some cases our synthetized carbosilane dendrimers (CBS-DDMs) reported low *in vitro* and *in vivo* toxicity and were able to effectively deliver the functional siRNA into the cells, release it into the cytosol and finally were able to achieve gene silencing of targeted gene. [2, 3, 4]

Research highlights

1) carbosilane dendrimers
2) transfection
3) gene therapy
4) non-viral vectors

References

[1] Miele, E. et al. 2012. Nanoparticle-based delivery of small interfering RNA: challenges for cancer therapy. Int J Nanomedicine 7: 3637-3657.

[2] Strasak, T. et al. 2017. Phosphonium carbosilane dendrimers for biomedical applications - synthesis, characterization and cytotoxicity evaluation. RSC Advances 7: 18724-18744.

[3] Liegertova, M. et al. 2018. Evaluation of toxicological and teratogenic effects of carbosilane glucose glycodendrimers in zebrafish embryos and model rodent cell lines. Nanotoxicology: 1-22.

[4] Herma, R. Et al. 2019. Carbosilane dendrimers with phosphonium terminal groups are low-toxic non-viral transfection vectors for siRNA cell delivery. International Journal of Pharmaceutics. 562: 51-65.

Xenografts in Zebrafish and dendrimers as drug delivery system

*Nejedla, Z[a]., Liegertova, M[a]., Herma, R[a]., Smejkal, J[a]., Maly, J[a].

[a]*Department of Biology, J.E. Purkyně University, Českе mladeže 8, 40096 Usti nad Labem, Czech Republic*

**presenting author, email: nejedla.z@email.cz, 2nd year of study*

Introduction

While a convencial approach in cancer therapy brings many side effects, the concept of targeted
drug delivery system (DDS) can open new possibilities in this filed. The approach of targeted DDS should be opened by a new nanostructures called dendrimers. Carbosilane dendrimers used in our experiments are the new type of nanoparticles with several different modifications, which should be able to fix and deliver drug to the target tissue. This property we will use *in vivo* after xenotransplantation of human adenocarcinoma of lungs to Zebrafish.

Material and method

In our experiments were used carbosilane dendrimers with NMe_3, PMe_3, $P(Et_2)_2(CH_2)_3OH$, Pbu_3, $P(C_6H_4\text{-}Ome)_3$, and $P(Ph)_3$ periphery substituents for *in vivo* tests. There was used a Fish Embryo Acute Toxicity (FET) Test established by OECD1 with *Danio rerio* embryos. For five days were embryos in chorion incubated in 28°C in dendrimers solution of concentrations 100μM, 10μM, 1μM, 0,1μM, 0,001μM plus positive and negative control. Four lethal-end points as a cogulation, lack of somite formation, lack of tail detachment from the yolk, heart oedema or lack of heartbeat were recorded by a microscope every 24 hours.

Results and discusion

The lowest toxicity has a phosphonium dendrimer (PMe_3). Embryos incubated in this type have as good viability as negative control till concentration 1μM, while dendrimers $P(Ph)_3$ and Pbu_3 has in concentration 1μM 100% mortality. All tested dendrimers have 100% mortality in concentrations 10μM and 100μM. Results of toxicity test help us to choose a good candidate and concentration for other experiments including the treatment of tumours caused by a transplantation a xenografts of human adenocarcinoma of lungs to *Danio* embryos. Xenotransplantation od CRL cells stained by a fluorescent tracker dye to embryos will be made by a mikroinjection into a yolk sac. The tumourgenesis will be analyzed by a volume measurment of each single tumour distributed to body. These results should be compared with tumour development in individual treated by a dendrimerdrug conjugate. The connection of dendrimer and tumor should based on We suppose dendrimers should be able to deliver the drug directly into a tumour based on the overexpression of EGFR receptors in this tumours type structures and the connection with the ligand on the perifery branches of dendrimer.

Conclusions

Dendrimers are a good candidates for targeted DDS, because of a possibility to make many modifications and commonly design it for many reactions and connections on really high specific level. These property determine their big potential for using in cancer therapy.

Research highlights

Nanotechnology in Biomedicine, Danio and Cancer Research, Drug Delivery Systém

1 [OECD Guidelines for the Testing of Chemicals 236], (2013)

Research was supported by project 2018-53-005-3 Internal Grand Agency UJEP.

Application of drones for monitoring the troposphere quality

*Pilnaj Dominik[a], Kuráň Pavel[a]

[a] *Faculty of the Environment, UJEP, Králova Výšina 7, Ústí nad Labem, 400 01, Czech republic*
**Ing. Dominik Pilnaj (1st year), dominik.pilnaj@ujep.cz*

The pollution of the troposphere has a major impact on the health of the Environment. Despite the effort to reduce emissions at source, there may be situations where immision limit values are exceeded. These situations can be studied with drones that are significantly more flexible than today's automatic air pollution monitoring stations. On the other hand, recent studies reveal the importance and complexity of natural volatile organic compounds and their meaning in the ecosystems. This field of research deserves attention due to the possibility to diagnose the condition of target ecosystem and taking early precautions.

The developed semi-automatic atmospheric sampler based on open-source technology is mounted with various sensors capable of feeding the atmospheric parameters to the remote server in real time with high frequency which allows online access with the possibility to construct detailed heat maps.

Detected parameters include temperature, humidity, pressure, gas flow. Concentration of several inorganic gases (SO_2, NO, NO_2, O_3) is measured by electrochemical sensors with limits of detection (LOD) at 10 $\mu g/m^3$. Dust particles PM 1, 2.5 and 10 will be analyzed by light scattering. Organic compounds are detected by photoionization detector with LOD at 10 $\mu g/m^3$. This sampler is also equipped with sorption tubes (possibly SPME arrows) for qualitative and accurate quantitative analysis of the atmospheric VOC by GC(xGC)-qTOF-HRMS.

The developed sampler might be used by organizations interested in the air quality (health institutes, regional authorities, …), industry (searching for leaks, work safety, …) or research institutions interested in the study of natural VOC.

Research highlights

1) Hardware and software development
2) Validation of the system according to ČSN
3) Research of various atmospheric pollution and its spread with subsequent risk evaluation
4) Research of natural VOC and their meaning in the ecosystems

References

[1] M. N. Norzailawati, A. Alias, R. S. Akma. *Designing zoning of remote sensing drones for urban applications: a review.* The International Archives of the Photogrammetry, Remote Sensing and Spatial Information Sciences, XLI-B6, (2016), 131 – 138.

[2] D. Gallacher. *Drones to manage the urban environment. Risks, rewards, alternatives.* Journal of Unmanned Vehicle Systems (dosud nevydáno).

[3] Ch. Chang et al. *A study of atmospheric mixing of trace gases by aerial sampling with multirotor drone*. Atmospheric Environment 184 (2018) 254 – 261.

[4] ČSN EN ISO 16017-1 (83 5741) Vnitřní, venkovní a pracovní ovzduší. Odběr vzorku těkavých organických sloučenin sorpčními trubicemi, tepelná desorpce a analýza kapilární plynovou chromatografií.

[5] ČSN ISO 4226 (83 5011) Kvalita ovzduší. Obecná hlediska

Bioavailability of elements in lingo-cellulose matrix

Zdeňka Kwoczynski*[a,b]

[a] *Faculty of environment, Jan Evangelista Purkyně University, Králova výšina 3132/7 400 96, Ústí nad Labem, Czech Republic*
[b] *Unipetrol centre of research and education, Revoluční 84 400 01, Ústí nad Labem, Czech Republic*
**presenting author, e-mail: zdenka.kwoczynski@unicre.cz, 2nd year of study*

My thesis deals with utilization of various biomass wastes with aim to create new product which can be used as fertilizer. Main aim of this work is a description of bioavalibility of nutrient contained in biomass wastes by plants. Nowadays, biowaste was burned or composted only. Burning of biomass is accompanied by CO_2 emissions and leads to loss of contained nutrients. The utilization of biomass for biochar production seems to be an efficient and environmentally friendly way of treating. Biochar is produced from biomass by low temperature pyrolysis [1]. The produced biochar is usually used as a sorption material [2]. Biochar can improve soil properties, e.g. retain moisture and cause aeration and with water also retains dissolved nutrients [3]. Biochar is very useful for a rich microbial growth in soils. Biochar is produced from various biomass wastes, e.g. corn, rice or bamboo [1, 3]. My work deals with wastes arising in the Czech Republic. In total, 12 different biomass wastes have been characterized. Digestate is a biomass waste that is produced on biogas plants. It contains a large amount of nutrients (N, P, K) and organic matter. Direct field spray of digestate is limited by a number of restrictions and problems [4]. The digestate contains a large amount of ammonia and methane, which are emitted into environment during spraying and can archive phytotoxic values and also causes losses of ammonia [5]. Recent research has shown that digestate is poorly biodegradable. Digestate stabilization by mixing with biochar would solves the problems and would occur the fixing the ammonia into the biochar would allow it to be incorporated into the soil. After finding a suitable source of waste biomass for biochar production, is necessary an analysis, especially chemical composition and surface analysis of biochar. For sorption of digestate, is advantageous high surface of biochar. That can be increased by activation. Biochar, digestate and their mixture will be added to the soil and a pot test on lettuce in greenhouse will take place. At the end of the experiment, soil samples will be taken for total elemental analysis and sequential extraction. After harvesting the lettuce, above-ground portion will be weighed and the root system evaluated. After evaluation of results of element analysis and lettuce grown, benefits of biochar and digestate addition should be proved.

Research highlights

1) Characterization of biomass wastes, which is produced in the Czech Republic and would be suitable for biochar production. Simulation of biochar production by TGA.
2) Biochar activation and detailed surface analysis (BET, SEM, potentiometric titration).
3) Pot tests with addition of biochar, digestate and their mixture. Subsequent elemental analysis of soils (focus on nutrients). Comparing total content and bioavailable fractions.
4) Evaluation of the influence of biochar, digestate and their mixture on the growth of plants.

References

[1] H. Wang et al., Bioresource Technology. 263, 2018, 444-449.
[2] D. Chen et al., Energy Conversion and Management. 169, 2018, 228-237.
[3] A. El-Naggar et al., Geoderma. 337, 2019, 536-554.
[4] V. Tigini, et al., Science of The Total Environment. 2016, 551-552,
[5] C. Da Ros et al., Ecotoxicology and Environmental Safety, 150, 2018, 150, 26-33

First results of *Miscanthus x giganteus* root exudates analysis

*Burdová H.[a], Trögl J.[a]

[a] *Faculty of Environment, J. E. Purkyně University, Králova výšina 3132/7, 400 96 Ústí nad Labem, Czech Republic*

**Ing. Burdová Hana, hana.burdova@ujep.cz, 2nd year*

Root exudates are substances which are secreted by roots into rhizosphere which is highly dynamic interface between roots and soil and as well as between roots and soil microorganisms. It is complex mixture of different organic substances, for example sugars, amino acids, organic acids, enzymes. The root exudates attract the benefical soil microorganisms, defend plant against pathogens [1] and they also play important role in the process of degradation [2]. The aim of this work is to analyse known and identify unknown root exudates of *Miscanthus x giganteus (Mxg)* which is well known for its ability to grow on contaminated soil [3] and high biomass production for non-food purpose [4].

There were taken *Mxg* plants grown in different types of matrices: soil and agar medium. First step was to optimize methods for collection and extraction of the substances. The direct probe interface with mass spectrometry, liquid chromatography with mass spectrometry and gas chromatography with mass spectrometry were used for analysis and identification of root exudates.

The pot experiments for studying impact of different contaminants on root exudates *Mxg* were established in May 2019. The soil was contaminated with diesel, polyaromatics hydrocarbons (phenanthrene, anthracene) and metals (cadmium, lead).

Research highlights

1) Isolation of root exudates *Miscanthus x giganteus*
2) Analysis of known root exudates of *Miscanthus x giganteus*
3) Identification of unknown root exudates of *Miscanthus x giganteus*
4) Correlation between the root exudates and different contaminated soil

References

[1] RUGOVA, A., et al. Elucidating rhizosphere processes by mass spectrometry - A review. *Anal. Chim. Acta*, 2017, vol. 956, p. 1–13.

[2] AMIR, H., et al. Rhizosphere engineering Enhancing sustainable plant ecosystem productivity. *Rhizisphere*, 2017, vol. 3, p. 233–243.

[3] PHANM NAM, H., et al. Influence of metal contamination in soil metabolic profiles *of Miscanthus x giganteus* belowground parts and associated bacteria communities. *Applied Soil Ecology*, 2018, vol. 125, p. 240–249.

[4] TÉCHER, D., et al. Contribution of *Miscanthus x giganteus* root exudates to the biostimulation of PAH degradation: An in vitro study. *Sci. Total Environ.*, 2011, vol. 409, p. 4489–4495.

POSTERY

A general hydrogen bonding definition based on three-dimensional spatial distribution functions and its extension to quantitative structural analysis of solutions and general intermolecular bonds

*Jan Dočkal[a], Martin Svoboda[a,b] ,Martin Lísala,[b], and Filip Moučkaa,[b]

a *Department of Physics, Faculty of Science, J. E. Purkinje University, Ústí n. Lab. 400 96, Czech Republic*

b *Department of Molecular and Mesoscopic Modelling, Institute of Chemical Process Fundamentals of the CAS, v. v. i., 165 02 Prague 6-Suchdol, Czech Republic*

**Jan Dočkal, e-mail: jan-dockal@seznam.cz*

Numerous microscopic definitions of hydrogen bonding have been proposed and employed in molecular simulations. They are typically based on various energetic, topological, and geometric criteria and require a specification of the cut-off values. The cutoff values are chosen to yield a reasonable description of hydrogen bonding in a particular molecular system under particular conditions and for a particular molecular model, and they are not thus straightforwardly transferable to different molecular systems or conditions. We propose a general approach to define and quantify the intermolecular bonds in liquids and solutions, including hydrogen bonds, which is free of any cutoff values. The approach is based on finding a continuous bond region in the surroundings of a local maximum of a spatial distribution function, enclosed by an isosurface going through the nearest significant saddle point. Moreover, the general definition of intermolecular bonding can quantify significance of particular intermolecular bonds or can be used locally to quantify and characterise bonds in heterogeneous systems or confinement. Besides the general definition of the intermolecular bonding, the bond region can be further characterised by a number of relevant properties such as the number of bonds per molecule, volume of a bond region per molecule, bond stability/strength or hydration number to provide deep insight into the intermolecular bonding. The approach is demonstrated for pure water and aqueous NaCl solutions under different thermodynamic conditions, and our results on the behaviour and quantification of their intermolecular bonding are compared with results obtained using commonly-used bond definitions.

Research highlights
1) Hydrogen bond
2) Molecular simulation
3) Spatial distribution function
4) NaCl, Structure

References
[1] J. Dočkal, M. Svoboda, M. Lísal, F. Moučka,. Journal of Molecular Liquids, 281, (2019), 225-235.

Selected classical and instrumental analytical methods for the nanomaterials characterization

*Jakub Ederer[a], Pavel Janoš[a], Petra Ecorchard[b], Michaela Šrámová Slušná[a,b],

[a]*Faculty of Environment, University of Jan Evangelista Purkyně, Králova Výšina 7, 400 96 Ústí nad Labem, Czech Republic*
[b]*Department of Materials Chemistry, Institute of Inorganic Chemistry AS CR v.v.i., Husinec-Řež Sq. 1001, 250 68 Řež, Czech Republic*

**Jakub Ederer, e-mail: Jakub.ederer@ujep.cz.*

Currently, it is important to describe properties, behavior in the environment and potential health risk of widespread types of materials resp. nanomaterials. For this purpose are commonly used sophisticated and complicated analytical methods (e.g. XPS, NMR, EXAF etc.). However there are still exist conventional analytical methods that are used in the last century however, today were replaced by HI-TECH methods mentioned above. Acid-base titration, electrochemistry, adsorption of the specific probe and FTIR can be categorized into the category of classical analytical methods. In the poster will be shown the versatility, simplicity and the possibility of the application of selected traditional analytical methods for characterization and description of selected nanomaterials like graphene oxide (Fig. 1, GO) and cerium oxide.

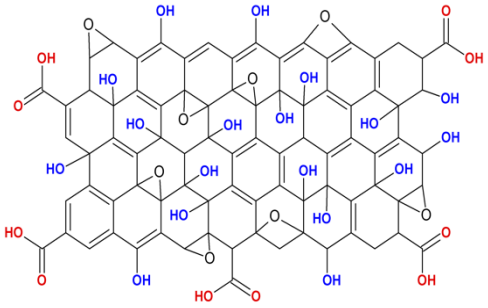

Figure 1 Structure of graphene oxide

Research highlights

1) Classical analytical methods
2) Acid-base titration
3) Graphene oxide, cerium oxide

References

[1] J. Ederer, et. al, *React. Funct. Polym.*, 2016, **103**, 44–53

[2] L. Forni, *Catalysis Reviews*, 1974, **8**, 65–115

Surface treatment of Al alloy by PTA of HSS30 steel

*Klára Jirounková[a], and Jaromír Cais[a]

[a] *Faculty of Mechanical Engineering, Institute of Technology and Materials, Pasteurova 7, Ústí nad Labem, Czech Republic*

**presenting author, e-mail: klara.jirounkova@ujep.cz (2)*

This research focuses on describing results of high speed steel upon the aluminium matrix surface by PTA surfacing method. The main motivation of this research has been an assignment of local company in order to prolong the lifetime of a tire press molds, especially the interface of its segments. These segmented molds are made from aluminium alloy and their interface is exposed to multiple percussions, which leads to cracks. Therefore, PTA surfacing is considered as a suitable surface treatment to harden its interfaces, yet benefit from lightweight of aluminium matrix. For purposes of this paper, the high speed steel HSS30 has been applied on the surface of Al-Si and alloy by PTA (plasma transferred arc) method. The PTA method has been developed as an improved plasma arc welding (protected by patent since the 50´s) for different materials in order to create so called Metal Matrix Composites [1]. These materials are subjected to different types of research focusing on its machining [2], corrosion resistance [3], interface between matrix and reinforcement [4] or comparison of different surface treatment effect [5] for over last 20 years. Since the PTA method brings a huge amount of energy into the process, material behavior is needed to be predicted. Their cohesiveness will be examined by confocal microscopy. Potential diffusion will be examined by EDX analyzer via element mapping in order to indicate the permeation of reinforcement with aluminium matrix.

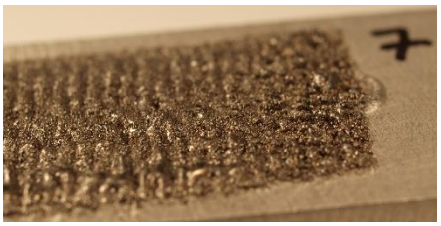

Figure 1 Reinforced Aluminium alloy by HSS30

Research highlights

1) The Al alloy reinforcement is widely demanded task since the millennium.
2) Metal Matrix Composites (MMC) can combine advantages of both materials.
3) Ferrous reinforcement can be deposited upon aluminium surface by PTA.
4) Their permeation can be indicated via element mapping by EDX analyser.

References

[1] Deuis R.L., Yellup J. M., Subramanian C. Metal-Matrix Composite Coatings by PTA Surfacing. Composites Science and Technology. 1998; 58. 299-309

[2] Durante S., Rutelli G., Rabezzana F. Aluminium–based MMC machining with diamond-coated cutting tool. Surface and Coating Technology. 1997; 94-95. 632-640

[3] Rodič P., Milošev I., Lekka M., Andreatta F., Fedrizzi L. Corrosion behaviour and chemical stability of transparent hybird sol-gel coatings deposited on aluminium in acidic alkaline solutions. Progress in Organic Coatings. 2018; 124. 286-295

[4] Rajan T. P. D., Pillai R.M., Pai B.C. Reinforcement coatings and interfaces in aluminium metal matrix composites. Journal of materials science. 1998 33. 3491-3503

[5] Ulutan M., Celik O.N., Gasan H., Er U. Effect of Different Treatment Methods on the Friction and Wear Behavior of AISI 4140 Steel. J. Mater.Sci.Technol. 2010; 26. 251-257

Grooved shaft analysis

* Pavel Kraus[a] , Klara Jirounkova[a] and Jaromir Cais[a]

[a] *Faculty of Mechanical Engineering, Institute of Technology and Materials, Pasteurova 7, Ústí nad Labem, Czech Republic*

**presenting author, e-mail: pavel.kraus@ujep.cz (5)*

Sample separated from the shaft (its grooved part) was delivered in order to be analysed. Examined part of the shaft was significantly corroded. Conducted analysis focuses on chemical composition analysis of delivered sample, documentation of teeth shapes in perpendicular section (exposed to corrosion) and chemical analysis of corrosion products. Fig. 1 shows examined sample (cut from grooved part of the shaft). In order to verify chemical composition of delivered sample, chemical composition analysis was conducted by using optical emission spectrometer. Standard chemical composition of steel given by standard ČSN 41 1523 was compared to measured values. Metallographic sample was subjected to macroscopic analysis of change in tooth curve by using stereomicroscope Olympus SZX 10. Also SEM Tescan VEGA 3 with EDX Bruker X-Flash was used to analyse surface of toothing and corrosion products. Examination of delivered sample lead to conclusions and recommendations for following usage.

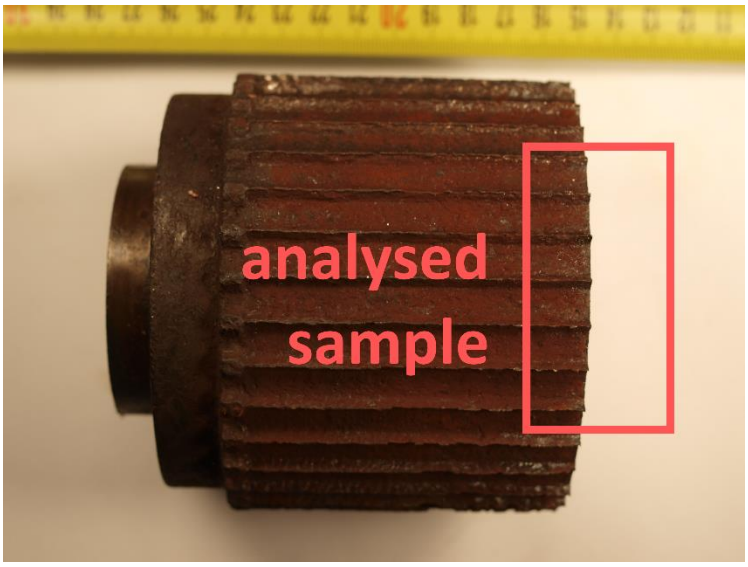

Figure 1 Analysed sample

Research highlights

1) Corrosion is a major issue for any industry involving iron and water.
2) It causes a significant decrease in material.
3) Decrease of material often leads to loose of a machine part function.
4) These kinds of machine part dysfunction can cause very expensive or dangerous.

Microbial and plant stress response during growing *Miscanthus x giganteus* in marginal lands: summary of first experiments

*Diana Nebeská[a], Hana Malinská[b], Josef Trögl[a] and Valentina Pidlisnyuk[a]

[a] *Faculty of Environment, Jan Evangelista Purkyně University in Ústí nad Labem, Králova výšina 3132/7, Ústí nad Labem, Czech Republic*
[b] *Faculty of Science, Jan Evangelista Purkyně University in Ústí nad Labem, České mládeže 8, Ústí nad Labem, Czech Republic*

**presenting author, e-mail: diana.nebeska@ujep.cz; 3rd year PhD study*

Miscanthus x giganteus (Mxg), C4 perennial grass, is under investigation as one of the most suitable crops for biomass production due to high biomass yields combined with low inputs requirements and other environmental benefits [1]. Thanks to its attributes it is good candidate for biomass production in marginal lands suffering from different problems (lack of nutrients, contamination etc.). It is able to grow in moderately heavy metals contaminated soils with slow phytostabilization of metals in root system. Few studies were published also about *Mxg* growing in PAH contaminated soils but generally potential for organic pollution phytoremediation with *Mxg* has not been fully studied yet [2]. Our goal was to investigate level of stress affecting *Mxg* plants growing in different marginal soils to better understand limits of *Mxg* phytotechnology application. Second task was focused on development of soil microbial communities as key factor of soil quality and health during *Mxg* cultivation.

For determination of plant stress non-invasive measuring of chlorophyll fluorescence was applied regularly during vegetation season and several indexes (e.g. Fv/Fm, performance index) indicating stress were calculated. Results of several pot experiments indicate that *Mxg* is stress tolerant to low level contamination with metals (Pb, Zn, Cu, Cd) but it is strongly affected by high petroleum pollution. Also significant deficiency of nutrients in sand soil was strongly limiting factor. State of soil microbial communities was examined using phospholipid fatty acids as indicator of living microbial biomass and for calculation of stress indicators. Additionally activity of selected extracellular enzymes was measured. Positive year-on-year effect on microbial community structure was determined during pot experiment in soils with elevated concentration of As, Cu, Sr, Zn and Zr. The same result was obtained for soil with increased Pb, Zn, Cu and Cd. In petroleum contaminated soil total microbial biomass was higher compared to control but significantly higher stress which was even increased year-on-year was revealed. Early results of field study in four different marginal sites in the Czech Republic suggest predominantly positive effect of *Mxg* rhizosphere on microbial enzymatic activity compared to non-cultivated soil and original vegetation.

Research highlights

1) *Mxg* is stress tolerant to heavy metals
2) Petroleum contamination and nutrient deficiency are strong *Mxg* stress factors
3) *Mxg* positively affects soil microbial communities in soil with heavy metals
4) *Mxg* rhizosphere supports microbial enzymatic activity in field conditions

References

[1] S. Arnoult, M. Brancourt-Hulmel. BioEnergy Res, 8 (2015), 502–526.
[2] V. Pidlisnyuk, T. Stefanovska, E. E. Lewis, L. E. Erickson, L. C. Davis. CRC. Crit. Rev. Plant Sci, 33 (2014), 1–19

Plasma modification of poppy seeds in fluidized bed reactor

*Jakub Perner

Faculty of science, Jan Evangelista Purkyně University, České mládeže 360/8, Ústí nad Labem Address, Czech republic

**Jakub Perner, p3rny@seznam.cz*

Adverse environmental conditions at planting, especially shortage of water can lead into reduced germination rate of seeds. Cold plasma treatment of seeds before planting can improve germination and make germs grow faster. Plasma discharge cause increase wettability of surface of seeds and disrupt the seed peel. This could lead to enhanced oxygen and water transport into the seed and improve germination conditions. [1] Seeds were treated in fluidized bed reactor in discharge of power from 10 to 40 W. Reactive gas was air at pressure 100 Pa. Poppy seeds were planted on 7 layers of filter paper saturated with water in petri dishes and the number of germinated seeds was observed from three to six days after planting. Every treated sample had improved germination rate compared to untreated (75,45 %) six days after planting. Highest rate had samples treated in discharge of power 40 W (81,21 %). Decrese of water contact angle on treated poppy seeds was observed from 85° (untreated) to 30 – 35° (treated). Untreated flax seeds has germination rate over 98 %. Research was focused on speed of germs growth. Treated seeds germs had only slightly higher weight than untreated, however water contact angle decreased from 99° (untreated) to 65 - 73° (treated).

Research highlights

1) Plasma treatment has positive effect on poppy seeds
2) Treated poppy seeds had almost 6% better germination rate
3) Treated poppy seeds had better wettability
4) Treated flax seeds growing process wasn´t significantly improved

References

[1] Sera, Bozena & Špatenka, P & Sery, Michal & Vrchotová, N & Hrušková, I. (2010). Influence of plasma treatment on wheat and oat germination and early growth. IEEE Transactions on Plasma Science. 38. 2963-2968.

Methane and carbon dioxide in dual-porosity organic matters: Adsorption and diffusion as seen from molecular simulations

Eliška Rezlerová[1,2] and Martin Lísal[1,2]

[1]*Department of Molecular and Mesoscopic Modelling, Institute of Chemical Process Fundamentals of the CAS, v. v. i., Prague, Czech Republic*

[2]*Department of Physics, Faculty of Science, J. E. Purkinje University, Ústí n. Lab., Czech Republic*

**presenting author, e-mail: Eliška Rerzlerová, 1st year of Phd studium, eliska.rezlerova@gmail.com*

Shale gas is an important unconventional energy resource that has had a potential game-changing effect on natural gas supply worldwide in recent years. Shale is comprised of two distinct parts: organic material and clay minerals. The organic material is primarily composed of kerogen but it also contains other compounds such as resin and heavy hydrocarbons. Clays are comprised of a large number of mineral particles arranged in piles of sheets. In shale formations, shale gas is stored as free gas, adsorbed gas and dissolved gas. The free gas gathers in the fractures and pores of a shale rock, the adsorbed gas occurs on the surfaces of both the organic material and clay minerals, and the dissolved gas enriches the organic matter.

We use an all-atom molecular dynamics simulation to generate the porous structures of mature and overmature type II organic matters with both microporosity and mesoporosity. We systematically characterise the porous organic-matter structures by calculating the geometric pore size distribution, pore limiting diameter, maximum pore size, accessible surface area, and pore volume. We then employ grand canonical Monte Carlo to study the adsorption of methane as a proxy of shale gas and equimolar methane/carbon dioxide mixture in the organic-matter structures. We complement the adsorption studies by simulating diffusion of methane, and methane/carbon dioxide mixtures in the organic-matter structures using molecular dynamics. Understanding of the properties of fluids in narrow pores found within shale formations and to develop atomistic/molecular scale models capable to predict fluid behaviour up to a mesopore and macroscopic (bulk) scale is critical for identifying ways to deploy shale gas technology with reduced environmental impact.

Research highlights

1) Monte Carlo simulation of CH_4 and CO_2 adsorption to kerogen
2) Molecular dynamics simulations of CH_4 and CO_2 diffusion in kerogen
3) Dual porosity molecular simulations of adsorption and diffusion

Multi-dimensional gas chromatography coupled with mass spectrometry (GC x GC-MS) for circular economy and environmental applications

M. Smaha[a], P.Kuráň[b]

Faculty of Enviroment, UJEP, Králova výšina 3132/7, Czech Republic

Mgr. Martin Smaha, Martin.Smaha@ujep.cz,(first year of study)

The aim of this work is to identify unknown organic compounds in pyrolysis products of waste materials. The work is mainly focused on the identification of green chemicals which are contained in these oils and are usable for further processing in various industries (chemical, pharmaceutical, food, etc.). These chemicals can replace or supplement feedstock industries and reduce the burden on the Environment.[1]

In particular, various waste materials of organic origin from plastics to wood waste will be used as feedstock for pyrolysis. These resources are subjected to pyrolysis to produce pyrolysis gas and pyrolysis oil, which will be subject of interest for further research. These oils contain many different chemical compounds from alkanes to sugars. [1] Due to the complexity of these substances, two-dimensional gas chromatography with mass detection (GCxGC-MS) will be used for characterization.[2] For pyrolysis oil samples, the application of several different techniques such as thin-layer chromatography (TLC), Sawadzky method and distilation will be used for separation. These methods are used for preseparation of compounds by differnt polarity or boiling point. [2,3]

Sawadzky method is a method where the oils are separated on a silica gel column using solvents with various polarity. The distillation method has the disadvantage of altering the original composition of pyrolysis oils and is therefore more suitable for separating fractions of certain boiling points and thein further analysis.[3]

After identification of the so-called green chemicals in pyrolysis oil, they will be separated by preparative chromatogramy in order to determine the purity of the product and estimation of its comercialization potential.[4]

Research highlights

1) Optimize methods of sample preparation and analysis of pyrolysis oils.
2) Identification of green chemicals in pyrolysis oils.
3) Extraction of green chemicals from this oils.
4) Analysis of isolated green chemicals and determination of their purity.

References

[1] MOHAN, D., PITTMAN, Ch. U., STEELE, P. H. Pyrolysis of Wood/Biomass for Bio-Oil: A Critical Review. *Energy & Fuels*, 2006, vol. 20/3, p. 848–889.

[2] TESSAROLOA, N. S., SANTOSB, L. R. D., RAPHAEL S.F., S., AZEVEDO, D. A. Chemical characterization of bio-oils using comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry. *Journal of Chromatography A*, 2012, vol. 1279, p. 68–75.

[3] NAIK, D. V., KUMAR, R., TRIPATHI, D., HEERES, H. J., KANAUJIA, P. K. Determination of the aging profile of pyrolysis oil derived from Apricot seed cake through solvent extraction and GC-MS analysis. *Energy Fuels*, 2017, vol. 31/11, p. 12297–12304.

[4] MICHAEL WINDT, M., MEIER, D., MARSMAN, J. H., HEERES, H. J., KONING, S. D. Micro-pyrolysis of technical lignins in a new modular rig and product analysis by GC-MS/FID and GC × GC-TOFMS/FID. *Journal of Analytical and Applied Pyrolysis*, 2009, vol. 80/2, p. 38–46.

Molecular dynamics study of racemic mixtures: Temperature dependence of separation of ibuprofen racemic mixture with β-cyclodextrin in methanol solvent

*Jiří Škvára[a], and Ivo Nezbeda[a,b]

[a] *Faculty of Science, J. E. Purkinje University, 400 96 Ústí nad Labem, Czech Republic*
[b]*Institute of Chemical Process Fundamentals, Acad. Sci. 16502 Prague 6 - Suchdol, Czech Republic*
**presenting author, e-mail: skvara.jiri@seznam.cz, year of study: 4.*

Active pharmaceutical ingredients are very often chiral molecules, with one enantiomer having the desired biological effect while the other being often even harmful. Methods for separation racemic mixtures or enantioselective synthesis used nowadays are costly or time consuming [1,2,3]. In the search for more efficient and cost-effective ways of obtaining optically pure, and thus less harmful, drugs, membrane separations seem to be very promising [4]. In a recent paper [5] we presented a computational model of chiral recognition using a membrane with β-cyclodextrin active site as a chiral selector for separation of (R)- and (S)-ibuprofen. At temperature 278.15 K differences in enantiomers affinity to β-cyclodextrin were found. However, from results of liquid chromatography it is known that the temperature dependence may be more pronounced and may thus affect the separation considerably [6].

In this work we present therefore a molecular simulation study of temperature dependence of separation of ibuprofen racemic mixture with β-cyclodextrin in methanol solvent. Cyclodextrine molecules are either freely placed in the system or they are tethered on the solid surface and formed enantionselective wall. The interaction of different enantiomers of quest molecule with the chiral selector moiety is investigated by inspecting the average interaction energy, hydrogen bonding, and differences in structural orientation between ibuprofen enantiomers and β-cyclodextrin.

The obtained results may serve both experimentalists and theorists as a benchmark for the development of a coarse-grained model to study the role of the structure of molecules and their intermolecular interactions for separation of racemic mixtures.

Research highlights

1) Differences in the behavior of the (S)- and (R)-forms in the coordination shells of cyclodextrin
2) Non-monotonic temperature dependence
3) Maximum of the separation effect

References

[1] W. Noorduin and E. Vlieg, Angew Chem., 48, (2009), 9600-9606
[2] A. Younes, H. Ates and D. Mangelings, J. Pharm. Biomed. Anal., 75, (2013), 74-85.
[3] J. Holaň , F. Štěpánek and L. Ridvan, Chem. Listy, 108, (2014), 46-49.
[4] C. Daniel, A. M. Rubio, P. J. Sebastião, C. A. M. Afonso, J. Storch, P. Izák, C. A. M. Portugal and J. G. Crespo, J. Memb. Sci., 505, (2016), 36-43.
[5] J. Škvára, I. Nezbeda, J. Mol. Liq., 265, (2018), 791-796.
[6] W. M. Ferrari, A. C. Nascimento, J. V. Moreira, M. A. Cremasco, Chromatogr. Res. Int., 2016, (2016), 1-6.

The influence of the preparation method of Cerium oxide nanoparticles on its properties

*Jakub Tolasz[a,b], Jiří Henych[a,b], and Pavel Janoš[a]

[a]*Faculty of Environment, Jan Evangelista Purkyně University in Ústí n. L., Czech Republic*
[b]*Institute of Inorganic Chemistry of the Czech Academy of Sciences, Husinec-Řež, Czech Republic*

**presenting author, e-mail: tolasz@iic.cas.cz*

Cerium oxide is a relatively widespread material with many applications in the industry, for example polishing or scouring of glass [1]. It is also the most important heterogeneous catalysts [2]. In recent years, its interactions with biologically relevant systems and related applications in medicine [3], have been extensively investigated. These applications of cerium oxide are usually based on the use of so-called nanocrystalline forms of cerium oxide (nanoceria). For these materials, which are able to mimic the effects of enzymes in living organisms, the term inorganic enzymes or nanozymes is used [4]. Several processes for the preparation of active forms of cerium oxide have been developed at the workplaces of UJEP and UACH. Some of these forms have the ability to decompose highly toxic compounds such as organophosphorus pesticides [5] or even structurally similar neural paralytic chemical warfare agents such as sarine, soman or VX [6]. Synthesis at low temperature (below 100°C) without further annealing was used in this work. Some samples have been prepared and characterized by physico-chemical methods such as XRD, XPS, DTA, BET and HRTEM. The aim was to find the relationship between the cerium oxide production process, its physicochemical properties and its degradation activity of parathionmethyl, which was measured by HPLC-DAD.

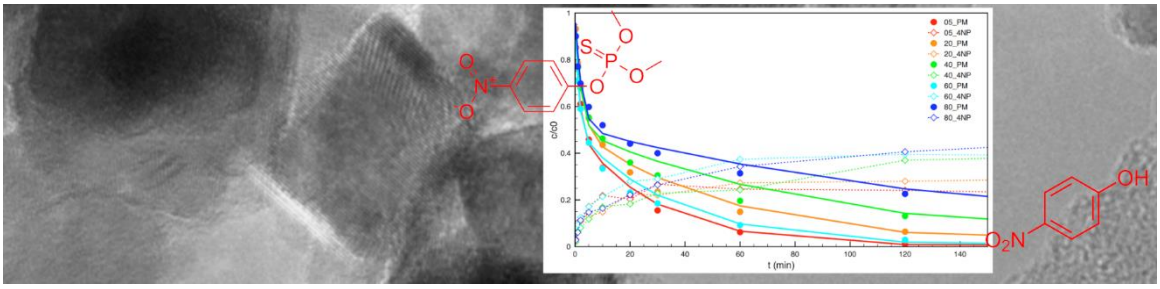

Figure 1 Degradation kinetics of parathionmethyl on surface of $nCeO_2$ particles.

Research highlights

1) Direct synthesis at low temperature below 100°C without annealing.
2) Monitoring of relationship between production process and application.

References

[1] P. Janoš, J. Ederer, V. Pilařová, J. Henych, J. Tolasz, D. Milde, T. Opletal, Wear. 362–363 (2016) 114–120.
[2] M.J. Manto, P. Xie, C. Wang, ACS Catal. 7 (2017) 1931–1938.
[3] T. Yao, Z. Tian, Y. Zhang, Y. Qu, ACS Appl. Mater. Interfaces. (2019).
[4] A.A. Vernekar, T. Das, G. Mugesh, Angew. Chemie - Int. Ed. (2016).
[5] P. Janos, P. Kuran, M. Kormunda, V. Stengl, T.M. Grygar, M. Dosek, M. Stastny, J. Ederer, V. Pilarova, L. Vrtoch, J. Rare Earths. 32 (2014) 360–370.
[6] J. Henych, V. Štengl, A. Mattsson, J. Tolasz, L. Österlund, J. Hazard. Mater. 359 (2018) 482–490.

Comparison of stream and floodplain sediments for identification of individual sources of pollution in fluvial system (Panenský Creek, Czech Republic)

*Štěpánka Tůmová[a,b] and Tomáš Matys Grygar[a,b]

[a] *Faculty of Environment, J.E. Purkyně University, Ústí nad Labem, Czech Republic*
[b]*Institute of Inorganic Chemistry AS CR, v.v.i., Řež, Czech Republic*

**Štěpánka Tůmová, 4th year, e-mail: stepatumova@seznam.cz*

Several pollution sources have acted along the Panenský Creek (an important tributary of the Ploučnice River): a facility for waste processing and recycling in Rynoltice (formerly a part of Czechoslovak Uranium Industry), lead-glass processing factory in Jablonné v Podještědí, and a Zn-plating factory in Brniště. The Ploučnice received most past pollution from large-scale U mining in Stráž pod Ralskem about half century ago. For the contamination assessment I combined floodplain and stream sediments analysis, geographical information systems (GIS) and gamma spectrometry dating based on ^{210}Pb and ^{137}Cs.

I sampled floodplain sediments for pollutant depth profiles and stream (channel bed) sediments for longitudinal pollution profiles. The samples were analysed using X-ray fluorescence spectrometry (XRF). Pollutant concentrations were evaluated in the form of their ratios to Fe a Ti concentrations (geochemical normalization) and these were compared with the Earth crust composition [1] to assess pollution levels.

Monitoring strategies for contaminated stream sediments frequently include unsubstantiated steps and neglect relevant aspects, such as sediment reworking and sediment composition control by its grain size. We used manual sampling in river channels, sieving, XRF analysis and analysis of particle size distribution (PSD) to evaluate the performance of geochemical normalization [2]. The aim was to improve that state and remove redundant steps that make research more time-consuming and potentially introduce biases.

For the normalization of Pb and Zn concentrations in the channel sediments, Fe concentrations are more suitable than Ti, probably because Fe oxides are carriers of most Pb and Zn and thus Fe, Pb, and Zn moves jointly in the channel. Contrarily, in the floodplain sediments, Fe is more mobile, in depths of typically fluctuating water table Pb and Zn ions are partly detached from Fe and then Ti is much better performing normalizer. If channel and floodplain sediments are compared, both Fe and Ti normalization must be used.

Research highlights

1) The Panenský Creek has been polluted by Zn and Pb from local factories
2) Pollution by Pb is still spread through the river system
3) The Panenský Creek is now more polluted than the Ploučnice River
4) Geochemical normalization with Fe and Ti can replace sediment sieving

References

[1] Rudnick R., Gao S., Composition of the continental crust. In: Rudnick, R.L., Holland, H.D., Turekian, K.K. (Eds.), The CrustTreatise on Geochemistry 3. Elsevier–Pergamon, Oxford, pp 1–64, 2003.

[2] Tůmová Š., Hrubešová D., Vorm P., Hošek M., Matys Grygar T., Common flaws in the analysis of river sediments polluted by risk elements and how to avoid them: case study in the Ploučnice River system, Czech Republic, Journal of Soils and Sediments, Volume 19, Issue 4, pp 2020–2033, doi: 10.1007/s11368-018-2215-9, 2018.

3D Spheroids for personalized approach in cancer therapy

*Žmudová, Z[a] ., Wróbel, D[a]., Herma, R[a]. , Malý, J[a].

Department of Biology, J.E. Purkyně University, České mládeže 8, 40096 Usti nad Labem, Czech Republic

**Presenting author, email: zuzana.zmudova@gmail.com, 2nd year of study*

Introduction

Personalized approach of cancer therapy based on 3D spheroids offers a possibility of extensive analysis of the molecular characteristics of tumor cells and tumor sensitivity assays to various available drugs. One of the ways to emulate tumor tissue is 3D cell cultures in this case so-called 3D tumor spheroids. The effect of drugs observed on 3D cultures is often very different from the effects observed in 2D culture and is very close to the actual effect of the drug on the tumor *in vivo*. With these 3D structures we tested the function of dendrimers, which were tested on 2D culture too.

Material and method

Test of cytotoxicity was made. For the cell viability assay were used three different cell lines - B14, NRK and BRL. There were analyzed six dendrimers types in three generations (G1-G3) measured by the same methods – MTT and CV. Every cell line was exposed to concentration gradient. For culturing of 3D spheroids were used cell lines MCF-7 and CRL. In three days is possible to observe spheroids. In the first step was made a test of toxicity on these spheroids with a nanostructure with drug delivering potential called dendrimers. Spheroids were monitored for 4 days and their growth was analyzed by a measurement of their volume. The toxic effect of dendrimer was evaluated using growth curves and analysis of ATP production by the luminescence method using CellTiter-Glo® Luminescent Cell Viability Assay.

Results and discussion

Cytotoxicity of PMe3 was similar or slightly lower as compared to NMe3 dendrimers. The highest toxicity of Pbu3 on 2D model was detected. Dendrimers with lowest cytotoxicity were P(Et2)2(CH2)3OH and P(Ph)3 . Also was observed their accumulation in mitochondria. Their low toxicity was confirmed by tests on 3D spheroids too. Therefore, both dendrimers could represent unique drug deliver systems for mitochondria targeting.

Conclusions

Toxicity of these two dendrimers P(Ph)3 and P(Et2)2(CH2)3OH are already tested on the 2D cultures and 3D spheroids. Results of both models will be compared.

Research highlights
3D Cultures, Personalized Therapy, Spheroids as Biomedecine Tool

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