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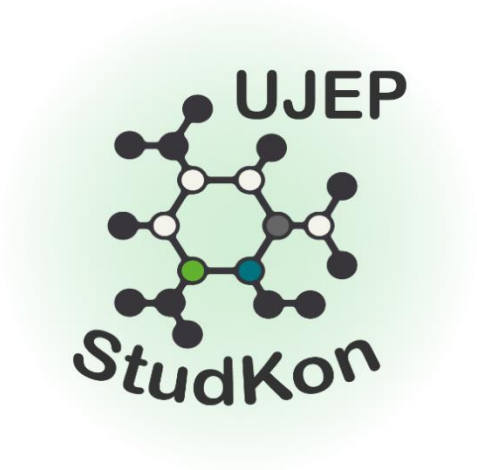

KNIHA ABSTRAKTŮ

Konference studentů přírodovědných a technických oborů UJEP

StudKon 2020

29. 6. 2020

Aula FŽP UJEP, Ústí nad Labem

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PROGRAM KONFERENCE

PONDĚLÍ 29. 6. 2020	
Registrace	**8:00 – 9:00**
Dopolední program	**9:00 – 13:20**
9:00 – 9:10	Zahájení a přivítání účastníků
9:10 – 10:30	Přednáškový blok 1
10:30 – 11:00	Coffee break
11:00 – 12:20	Přednáškový blok 2
12:20 – 13:20	Polední přestávka – oběd, instalace posterů
Odpolední program	**13:20 – 19:00**
13:20 – 14:10	Krátké představení posterů
14:10 – 14:40	Vystoupení hosta konference
14:40 – 15:10	Coffee break
15:10 – 16:30	Přednáškový blok 3
16:30 – 18:00	Posterová sekce
18:00 – 19:00	Technická přestávka
Večerní program	**19:00 – 22:00**
19:00 – 19:30	Vyhlášení výsledků soutěže o nejlepší poster a přednášku, a soutěže o nejoriginálnější příspěvek, vystoupení rektora univerzity a hostů
19:30	Večeře / raut
20:00 – 22:00	Společenský program, během něj budou vyhlášeny výsledky studentské soutěže, ukončení konference

PŘEDNÁŠKOVÝ BLOK 1 (9:10 – 10:30)

Michal Hošek: Environmental threat of the worst Hg pollution hotspot in central Europe (9:10)

Štěpánka Tůmová: Geochemical properties and background functions of floodplain sediments of the Panenský Creek (Czech Republic) (9:30)

Diana Nebeská: Activity of soil microorganisms during Miscanthus x giganteus cultivation: first results of the field study in the Czech Republic (9:50)

Zuzana Žmudová: EGFR siRNA inhibition gene therapy in 2D and 3D cultures (10:10)

PŘEDNÁŠKOVÝ BLOK 2 (11:00 – 12:20)

Jiří Smejkal: Recombinant proteins as a substitute for antibodies in microfluidic chips for cell immunocapture (11:00)

Petr Aubrecht: Preparation and characterisation of silan based surfaces for use in 3D tumor spheroid culture (11:20)

Adéla Jagerová: High energy Au+ ion implantation of polar and nonpolar ZnO - Structural modification and optical properties (11:40)

Martin Šťastný: Nanostructured manganese oxide-based catalysts: Comparison between assisted hydrolysis of bis(4-nitrophenyl)phosphate (BNPP) and catalytic decomposition of methanol (12:00)

PŘEDNÁŠKOVÝ BLOK 3 (15:10 – 16:30)

Jan Hubáček: Pyrolysis of plastic waste – process optimization, product analysis and dehalogenation (15:10)

Eliška Rezlerová: Methane and carbon dioxide in dual-porosity organic matter: molecular simulations of adsorption and diffusion (15:30)

Martin Kozakovič: Vertical bladed mixer: the analysis of polydisperse granular media flowing (15:50)

Jan Dočkal: Molecular force field development for aqueous electrolytes (16:10)

POSTEROVÁ SEKCE

Burdová Hana	The impact of diesel pollution on growth Miscanthus x giganteus
Herma Regina	Study of biological effects of new types of carbosilane dendrimers
Kaule Pavel	Direct lithiation-halogenation of metallacarborane cluster
Lupínková Simona	Sulphur particles immobilized on activated polymer surface
Nejedlá Zuzana	Class II biocompatible E-shell 300 3D printing material causes severe developmental toxicity in Danio rerio embryos - implications for 3D printed microfluidics
Panuška Petr	Microfluidic fish embryo test chip with the ability to remove individual eggs during long-term cultivation
Perner Jakub	Plasma treatment of poppy seeds in fluidized bed reactor
Pilnaj Dominik	Application of drones for tropospheric quality monitoring
Poustka David	Nanofibrous and nanostructured materials for biomedical microfluidic devices
Ryšánek Petr	Specific structure, morphology, and properties of polyacrylonitrile (PAN) membranes prepared by needleless electrospinning; Forming hollow fibers
Štojdl Jiří	New equipment constructed for bathymetry mapping at the Faculty of the Environment
Tolasz Jakub	Room-temperature synthesis of nanoceria for degradation of organophosphate pesticides and its regeneration and reuse
Wildová Eliška	Seasonal accumulation of manganese content in plant species of forest ecosystem affected by anthropogenic activities

Přednáškový blok 1
(9:10 – 10:30)

Environmental threat of the worst Hg pollution hotspot in central Europe

*M. Hošek[a,b], T. Matys Grygar[a,b], J. Štojdl[a] , J. Svoboda[a]

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Rivers and their surroundings are usually perceived as a symbol of nature and purity. Unfortunately, in the last centuries rivers have been linked with heavy industry. The river channels and floodplains have thus become contaminated by wastes of all kinds, frequently being hazardous to humans. With Hg, this risk is even higher due to its extraordinarily high toxicity. Inorganic forms of Hg can easily be methylated by bacteria into a neurotoxic species containing methyl-Hg (MeHg), which are bioaccumulated in food webs with potential harmful effects on aquatic organisms and subsequently for man.

This study has been conducted in the catchment of the Kössein and the Röslau rivers (Bavaria, Germany), polluted by Hg compounds from Chemical Factory Marktredwitz. The factory was closed after 200 years of operation 30 years ago due to an illegal discharge of waste straight into the Kössein River. Worrisome amount of Hg, ca. 20 t, is present in the 22 km long channel belt of the rivers in easily erodible sediments. Two questions are immediately born in mind: 1) is revitalization of the river system possible, and 2) what are the actual gateways of Hg to food chain in that hotspot. To answer these questions, we have described the pollution distribution and subsurface sedimentary architecture in one site of the hotspot.

We used geophysical methods ERT (electrical resistivity tomography) and DEMP (dipole electromagnetic profiling), supported by drill coring, *in situ* element analysis by handheld X-ray fluorescence spectroscopy (XRF), and *ex situ* Hg analysis of selected samples by AMA-254. Because Hg concentrations were frequently too low for XRF, we used close correlation between Zn and Hg (R^2=0.647) to recognize contaminated sediments. The sediments were classified into three types (*facies* in sedimentology terms) with different concentrations and the risk of their re-entering into the fluvial system. Most presented *channel belt sediments* (up to 122 mg Hg/kg) are prone to reworking under flood conditions. These sediments could also endanger aquatic life by the formation of water-soluble MeHg or transfer of Hg to food web via aquatic and littoral plants. *Fills of shallow flood channels* in floodplain (up to 73 mg Hg/kg) reflect ancient history of floodplain architecture, like abandoned meanders, but perhaps do not pose a particular risk for life. The *top strata of overbank fines* (up to 56 mg Hg/kg), representing layer of easily accessible contaminants for plants, should be mapped because of common use of floodplain as meadows for hay production and grazing.

Research highlights

1) Mercury pollution hotspot in floodplains in German-Czech border
2) Three distinct sedimentary facies were distinguished in studied floodplain
3) Each of the facies has a distinct Hg concentration and risk of physical mobilization
4) Channel belt sediments and overbank fines represent largest risk for biota

Geochemical properties and background functions of floodplain sediments of the Panenský Creek (Czech Republic)

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Pollution by lead and zinc was studied in approx. 30 depth profiles in the floodplain sediments of the Panenský Creek, an important tributary of the Ploučnice River, the Czech Republic. The Panenský Creek was impacted by several undocumented pollution sources acting in the 20th century, such as 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 River received most past pollution from large-scale U mining in Stráž pod Ralskem about half century ago.

For the pollution assessment, I sampled floodplain sediments for pollutant depth profiles (profile depth 1 – 2 m) and analysed them by X-ray fluorescence spectrometry (XRF). Unpolluted sediment samples were selected and processed to produce the local background functions, necessary to determine the natural concentration of risk elements with respect to local geology and subsequent evaluation of the anthropogenic pollution. The element concentrations must not include sediments affected by post-depositional migration related to reductomorphic processes and recrystallisation of Fe and Mn oxides driven by a fluctuating water table [1].

The observed concentrations of risk elements have been normalized. Due to eliminate the influence of the lithological variability on the sediment I used a geochemical normalization - calculation of the concentration ratios of risk elements (Zn and Pb) to normalizing element (Ti, Fe, Al, Rb). Each element was assessed separately due to the different effects of pollution sources. For Zn I found out the suitability of the normalizing element: Ti > Al > Fe > Rb. For Pb was: Rb > Ti > Al > Fe. All normalizations are statistically significant. Then I calculated of local enrichment factors (LEF) from them to assess pollution levels independent of sediment coarseness. Results were also compared with value of the Earth upper crust composition [2].

Research highlights

1) The Panenský Creek has been polluted by Zn and Pb from local factories
2) Grain-size control is suppressed by geochemical normalization
3) Assessment of background values and risk elements enrichment in floodplains
4) Concept of local enrichment factors based on local background functions

References

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Activity of soil microorganisms during *Miscanthus x giganteus* cultivation: first results of the field study in the Czech Republic

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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 a good candidate for biomass production in marginal lands suffering from different problems (lack of nutrients, contamination etc.) [2]. Our goal was to study effect of *Mxg* cultivation on activity of soil microorganisms as one the biological indicators of soil quality.

Mxg has been grown in three different fields in the Czech Republic which can be sorted as marginal. The cultivation lasted one or two vegetation seasons (years 2018 and 2019). The following sites were under investigation: the former military airport Hradčany with very low-quality sand soil (2019), low quality agricultural field in area with mining history in Chomutov (2018-2019) and the reclaimed part of landfill constructed above former coal mine in Ústí nad Labem – Všebořice (2018-2019).

In order to evaluate effect of *Mxg* cultivation on soil microorganisms four different soil samples were collected in each of the fields, i.e.: 1) rhizosphere soil closely attached to *Mxg* roots, 2) bulk soil, 3) field soil between *Mxg* plants and 4) non-cultivated soil behind the fields border with original vegetation. Activity of soil microorganisms was determined as basal soil respiration and activity of selected hydrolases (extracellular enzymes representing biogeochemical cycles of nutrients C, N, P and S).

The analysis showed that basal soil respiration was generally higher for Chomutov and Všebořice compared to Hradčany sandy soil. In the first year respiration in *Mxg* rhizosphere was significantly higher than other samples in Chomutov and Všebořice but in second year the rhizosphere activity was comparable and generally lower than in 2018, which may be caused also by different weather conditions before sampling in those two years. On the other hand, in Hradcany the soil respiration around *Mxg* roots was even lower than in surrounded field soil. Different behaviour of Hradcany and Chomutov soils was confirmed also by activity of hydrolases. While in Hradcany the highest activity was determined in samples from undisturbed area with original vegetation, in Chomutov and the highest values were in *Mxg* rhizosphere in both years.

Research highlights

1) *Mxg* effect on soil microorganisms activity is dependent on soil quality/type
2) In sand soil *Mxg* cultivation has negative effect on microbial activity at least in first year
3) In marginal soil with better nutrition the *Mxg* effect was mainly positive in first two years
4) Longer observation is necessary to determine *Mxg* long-term effect and climatic effects

References

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EGFR siRNA inhibition gene therapy in 2D and 3D cultures

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Chemical nanostructures called dendrimers have big potential in the field of nanotechnology-provided gene therapy. Dendrimers are promising as potential non-viral vectors to deliver siRNA for RNAi purpose due to their unique features based on the well-defined structure and the presence of several functionalizable peripheral groups. Although the various uses, the main investigations of complexes siRNA/dendrimer (dendriplex) is mostly focused on their binding behaviour with cells (2D cultures), but their applications in three dimensional (3D) cell culture, remains untouched.

Two cancer cell lines for two dimensional cells and three dimensional multicellular spheroids testing of siRNA delivery system were used. Adenoma cancer cells CRL known for their overexpression of EGFR and HTB cell line as a control. For spheroids formation, commercial 3D Petri Dish® was used. After 3 days of cultivation is possible to observe spheroids. As a carrier for siRNA molecule delivery against expression of EGFR was used phosphonium dendrimer. The cell viability was measured by fluorescence microscopy. The viability of spheroids and cells was evaluated by the luminescence method using CellTiter-Glo® Luminescent Cell Viability Assay.

Carbosilane dendrimers with PMe3, P(Et2)2(CH2)3OH, PBu3,P(C6H4-OMe)3 and P(Ph)3 peripheral substituent could be suitable for drug delivery system. Especially dendrimers with PMe3 and P (Et2)2(CH2)3OH peripheral substituent seems promising due to low cytotoxicity even at high concentrations. Dendrimer PMe3 was selected for gene therapy via siRNA against EGFR.

Research highlights

1) Differences in ATP production were observed between 2D and 3D cultures.
2) The cytotoxicity of carbosilane dendrimers with PMe3, P(Et2)2(CH2)3OH, PBu3, P(C6H4-OMe)3 and P(Ph)3 peripheral substituent was successfully tested.
3) Cell proliferation was significantly inhibited after EGFR siRNA exposure.

Přednáškový blok 2
(11:00 – 12:20)

Recombinant proteins as a substitute for antibodies in microfluidic chips for cell immunocapture

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The development of microsystems for cell-based studies is very demanding in biomedical research and has many possible applications, capturing rare and circulating tumor cells in particular. Most of the microfluidic devices for rare cell detection have been based on the immunophenotyping approach.

Novel approaches in the development of recombinant protein binders with high potential of replacing the traditional antibodies in diagnostic and therapeutic applications were successfully demonstrated. Despite their large application potential, there are only a few examples of protein binders use in biosensors or microfluidic diagnostic devices, based solely on protein binders [1].

To our best knowledge, all published papers related to protein binders application in medical diagnostic devices were, up to now, focused solely on the detection of soluble protein markers. Here, we bring the first proof-of-principle example of protein binders application in cell immunocapture microfluidic device. In cooperation with the Institute of Biotechnology of the Czech Academy of Sciences, we have developed brand new protein binders capable of recognizing IL-17R, IL-23R membrane receptors. Although initial testing showed that many protein binders can bind to the receptors in the cell suspension, only a couple of protein binders preserve its function after its immobilization on the planar surface, due to the conformation changes on the protein binders. Using unique stop-flow regime of the interrupted flow of fluid in our microfluidic device we have demonstrated the efficient THP-1 cell line capture in simple glass microfluidic device modified by REX and ARS protein binders targeting the IL-17R and IL-23R cell surface receptors with up to 70% capture rate, that can rival capture rate of traditionally used antibodies. Our protein binders and the microfluidic device could be exploited in designing microfluidic devices for immunochemical cell capture, including the rare cells and circulating tumor cells.

Research highlights

1) Dozens of newly synthesized and never before used proteins were tested for their capability to bind cells to the planar surface.
2) Protein binder capable of binding cells expressing IL-17R and IL-23R cell surface receptors to the planar surface was found.
3) In our application, protein binders can replace antibodies in microfluidic chips for cell immunocapture, making the application significantly cheaper.
4) The presented microfluidic device offers the possibility of integration into many medical devices, thanks to its easily exploitable design.

References

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Preparation and characterisation of silan based surfaces for use in 3D tumor spheroid culture

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In comparison with 2D cell culture models, 3D spheroids can accurately mimic some features of solid tumours, such as their spatial architecture, physiological responses, secretion of soluble mediators, gene expression patterns and drug resistance mechanisms [1]. These unique characteristics highlight the potential of 3D cellular aggregates to be used as in vitro models for screening new anticancer therapeutics, both at a small and large scale [1–3].

Formation of spheroids occurs spontaneously, in environments where cell-cell interactions dominate over cell-substrate interactions. Conventional methods for spheroid generation include hanging drops, spinner flask cultures, rotary cell culture systems and culture of cells on non-adherent surfaces [2].

This work is focused on the preparation and characterization of thin layers of silane compounds on the glass surface, for the use in the cultivation of 3D tumour spheroids in medical applications. Previously optimised parameters were used for the preparation of the silanized surfaces (APTES, MethylS, and PropylS) in this work.

The methodical part is firstly focused on the preparation of the surfaces and their characterization by given analytical methods (Contact Angle Measurement, XPS, Zeta Potential and AFM) and then on the preparation of silanized surfaces and their integration into the simple static microfluidic device for cell cultivation and viability testing.

Research highlights

1) Silanized glass substrates were characterized for the use as antifouling surfaces.
2) Trimethoxymethylsilane is showing greatest antifouling properties.
3) 3D tumour cell spheroids can be cultured on this surface with potential to be used in microfluidic device for anticancer therapeutics research.

References

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High energy Au^+ ion implantation of polar and nonpolar ZnO - Structural modification and optical properties

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Crystalline zinc oxide (ZnO) is a direct wide bandgap semiconductor popular in various optical and optoelectrical applications such as solar cells, light-emitting diodes or gas sensors. Doping of ZnO by noble metals like silver or gold and preparation of nanocomposite or nanoparticles can lead to a change in optical or catalytic properties [1, 2]. Approaches in ion implantation allow efficient synthesis of nanostructures or nanoparticles with precise control of dopant concentration and its depth distribution however it is accompanied by radiation damage with a negative effect on the crystal properties [3]. ZnO exhibits high radiation resistance and as well as GaN shows damage asymmetry for different crystallographic orientations, but the damage mechanism after high energy implantation is still not completely understood [4]. In this work, c-plane, a-plane, and m-plane ZnO were implanted with 5 MeV Au^+ ions with fluences $5x10^{14}$ and $1x10^{15}$ cm^{-2} for investigation of the damage formation mechanism of different crystallographic orientations. Further, modified ZnO samples were annealed with a temperature 600°C in the O_2 atmosphere to reach structural recovery. Rutherford backscattering spectrometry channelling (RBS-C), used for monitoring of crystalline changes, demonstrate significantly lower crystal damage for a-plane ZnO in both subsurface and implanted regions with small temperature recovery. RBS-C angular scans show a narrowing of channels after implantation in the subsurface region mainly for c- and m-plane ZnO. Information about crystal damage in different crystallographic orientations was completed with the Raman spectroscopy. Finally, the analysis of optical properties by a luminescence measurement shows dismissing of peaks or shift to shorter wavelengths after implantation. Annealing has a beneficial impact on a recovery of luminescent peaks and shift towards the higher wavelengths.

Research highlights

1) Modification of ZnO with energetic ions for optoelectronic applications
2) Study of radiation resistance of ZnO in different crystallographic orientations
3) Investigation of annealing effect on the ZnO structural recovery

References

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Nanostructured manganese oxide-based catalysts: Comparison between assisted hydrolysis of bis(4-nitrophenyl)phosphate (BNPP) and catalytic decomposition of methanol

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Manganese oxide-based (MnO_x) catalysts have received increased attention due to their low cost, low toxicity, and the ability to degrade organic molecules at low temperatures [1,2]. In this work, a series of four MnO_x-based catalysts was prepared by combination of homogeneous precipitation and redox reactions of manganese salts in an aqueous solution. A wide arsenal of analytical techniques, such as nitrogen physisorption, XRD, H_2-TPR, Raman, TEM, and XPS spectroscopies, were applied for their characterization. The nanostructured MnO_x exhibited high catalytic activity in hydrolysis of phosphate diester-based substrate (BNPP) at 55 °C. Furthermore, the MnO_x-based catalysts were also tested for partial oxidation of methanol (POM) reaction. It can be concluded that the varying abundance of redox-active $Mn^{2+}/Mn^{3+}/Mn^{4+}$ surface sites together with the high proportion of oxygen species (such as O^{2-}, or O^-) are significant to its high catalytic activity for the catalytic degradation of both molecules.

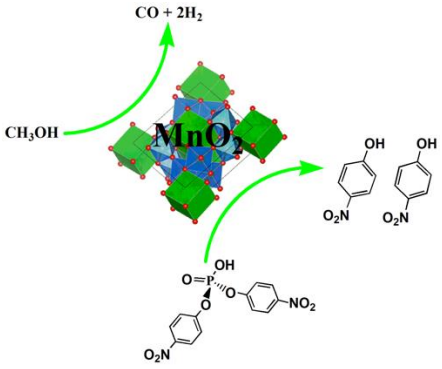

Figure 1 Scheme for catalytic decomposition of BNPP and methanol on the surface of MnOx catalysts.

Research highlights

1) Low-cost and straightforward synthesis of environmentally-friendly MnOx-based catalysts
2) High catalytic activity against assisted hydrolysis of BNPP and catalytic decomposition of methanol at low temperatures

References

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Přednáškový blok 3
(15:10 – 16:30)

Pyrolysis of plastic waste – process optimization, product analysis and dehalogenation

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Humanity is currently facing a number of challenges, such as global warming or waste management, where one option is to recycle waste and use renewable resources. Considering plastics, there is often problem with variability of these materials and mechanical recycling isn´t always viable option. Pyrolysis is an interesting way to obtain valuable products from these materials with potential further use in the refining and petrochemical industries [1]. However, this use is often hindered by the presence of halogens, which must be removed during the process or in subsequent treatments [2].

Pyrolysis of virgin polymers was conducted in batch laboratory unit with fixed bed. Individual polymers such as HDPE, LDPE, PP, PS, PVC and mixture of these polymers was pyrolyzed and respective products were analyzed with various methods. Several temperature programs were tested along with different residence times in order to maximize liquid product yield, improve its properties and decrease chlorine content. In addition, off-line experiments in autoclave were conducted with model chlorinated compounds and real pyrolysis oils from mixed plastics, in order to address further necessary dehalogenation. Chlorine content in liquids was analyzed with XRF and qualitative evaluation was made with various chromatographic techniques such as GCxGC-MS or GC-FID. Further research was proposed based on gathered data, both in laboratory and pilot scale.

Research highlights

1) Optimization of the pyrolysis unit for subsequent use of catalysts and sorbents for the treatment of pyrolysis products.
2) Thorough characterization of pyrolysis products with a focus on chlorinated substances.
3) Experiments in autoclave dealing with dehalogenation of model mixture and real pyrolysis liquid.

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Methane and carbon dioxide in dual-porosity organic matter: molecular simulations of adsorption and diffusion

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Shale gas, which predominantly consists of methane, is an important unconventional energy resource that has had a potential game-changing effect on natural gas supplies worldwide in recent years. The injection of carbon dioxide in the exchange of methane within shale formations improves the shale gas recovery, and simultaneously sequesters carbon dioxide to reduce greenhouse gas emissions. Laboratory experiments can provide only limited information about the adsorption and diffusion behaviour of fluids in shale pores because typically the experiments are performed under low to medium temperatures and pressures, which differ from realistic reservoir conditions. Molecular-level simulations are important alternatives and complementary tools to experimental measurements since they can provide detailed information about the microscopic mechanism of the gas adsorption/desorption and diffusion processes in the shale matrix at realistic reservoir conditions.

In this work, we apply molecular-level simulations to explore adsorption and diffusion behaviour of methane, as a proxy of shale gas, and methane/carbon dioxide mixtures in realistic models of organic materials (OM). We then employ the grand canonical Monte Carlo technique to study the adsorption of methane and the competing adsorption of methane/carbon dioxide mixtures in the OM porous structures. We complement the adsorption studies by simulating the diffusion of adsorbed methane, and adsorbed methane/carbon dioxide mixtures in the OM structures using molecular dynamics.

The total adsorption of pure methane, and to a certain extent the excess adsorption, increases with increasing pressure and decreases with increasing temperature. Also, its diffusion along the adsorption isotherms anti-correlates with the adsorption behaviour. In equimolar mixture of methane and carbon dioxide, CO_2 preferentially adsorbs compared with methane in the OM structures. The methane adsorption behaviour in the mixture is analogous to the pure methane adsorption behaviour. The CO_2 adsorption isotherms are affected by a sharp increase in the bulk density near the CO_2 critical pressure. Species diffusions along the mixture adsorption isotherms in general anti-correlate with the mixture adsorption behaviour.

Research highlights:

1) Realistic kerogen models were created and characterised to study CO_2 and CH_4 behaviour.
2) Monte Carlo method was employed to study the preferential adsorption of CO_2.
3) Species diffusions were simulated to explore the interplay between the adsorption and diffusion.
4) Species diffusions anti-correlate with the adsorption behaviour.

Vertical bladed mixer: the analysis of polydisperse granular media flowing

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The motivation of this research was to explore the competition between the homogenization and segregation processes of the polydisperse dry granular material in the cylindrical mixer. Our previous publishing activity was particularly focused on this transport problem (Barczi, 2018) in the rotating drum. The mixing was performed in a vertical cylindrical mixer with two opposed flat blades with a 45° rake angle. The computational simulation of the mixing process was performed for glass beads with 1, 2 and 4 mm diameter arranged in the axial (bottom-up), radial (side-by-side) and tangential (inside-outside) limit initial packing configurations. The values of the blades rotational speed were set to 150 and 15 revolutions per minute (rpm). The study was divided into two stages. The effect of particle size on the homogenization process was studied in the first stage. These results were used as a stepping stone for the examination of the segregation phenomenon in the next stage.

The level of homogeneity was evaluated by using mixing indexes in the first stage of the research. It was found out the homogenization process was negatively influenced for lower particle diameter. Deeper analysis shown this was caused by higher energy dissipation. The segregation was explored in the next stage of the research. The evolution of the particles flow for first 80 revolutions and 150 rpm is presented in the Figure 1. The initial position of particles with 4 mm diameter was set up in the bottom of the vessel. It can be seen particles were percolated to the top layer of the vessel after 10 revolutions. The stationary regime arose after 40 revolutions. In this case the system is divided into the segregated region at the top layer of the vessel and homogenized region in the middle of the vessel. Once the system is stabilized, the particles are no longer segregated. This phenomenon enables the segregation process can be controlled.

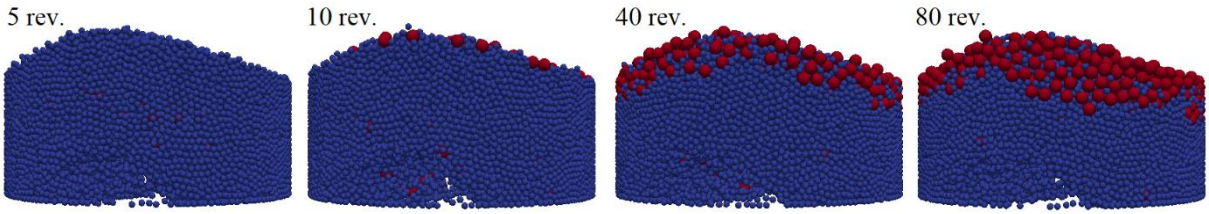

Figure 1. The visualization of the beads with the axial initial configuration. The initial position of particles with 4 mm diameter is the bottom of the vessel. The blades rotational speed is 150 rpm.

Research highlights

1) The lower the particle size is the worse the level of homogeneity occurs.
2) The system is no longer segregated in the stationary regime.

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Molecular force field development for aqueous electrolytes

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The current state-of-the-art force fields (FFs) for Na^+ a Cl^- ions are not capable of simultaneously predicting the thermodynamic properties of the aqueous solution and the crystalline phase. This is primarily due to an oversimplification of the interaction models used but partially also due to the insufficient parametrization of the FFs. We have devised a straightforward and simple parametrization procedure for determining the ion-ion interaction parameters in complex molecular models of NaCl electrolytes which involves fitting the density, lattice energy and chemical potential of crystalline NaCl at ambient conditions. Starting from the AH/BK3 and MAH/BK3 FFs, the parametrization approach is employed to develop a complex and accurate polarizable molecular model for the NaCl electrolyte by parametrizing the ion-ion interactions. The performance of the refined polarizable NaCl FF is assessed by evaluating the different thermodynamic and mechanical properties of the crystal, density of crystalline and molten NaCl along with the melting temperature, properties of aqueous solutions, and the structure and stability of hydrohalite. The simulation results confirm the superiority of the refined FF in comparison with the existing state-of-the-art FFs to accurately predict a wide range of system properties in different NaCl phases, including NaCl aqueous solubility.

Research highlights

1) A novel parametrization procedure for ion-ion interaction of NaCl is presented.
2) The procedure was used to develop a new polarizable force field for NaCl.
3) New model was succesfully tested on a large number of thermodynamic and mechanical properties.

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Posterová sekce

The impact of diesel pollution on growth *Miscanthus x giganteus*

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Energy crop *Miscanthus x giganteus* (*Mxg*) is well known for its ability to grow in contaminated soils and high biomass production as well as for possibility to be transformed to various biobased products [1,2].

A pot experiment was set to determine impact of diesel pollution on *Mxg* growth and impact of *Mxg* on degradation of diesel pollution. *Mxg* was grown in pots with diesel spiked soil with different concentrations (2 500 – 50 000 mg/kg). The soil parameters as pH, TOC and diesel concentration (C_{10} – C_{40} analysis) were monitored. The changes in the microbial community were evaluated by PLFA analysis and activity of soil microorganisms was determined by measurement of respiration and enzymatic activities (dehydrogenases and selected extracellular enzymes representing biogeochemicals cycles of important nutrients).

Research highlights

1) Impact of diesel pollution on growth of *Miscanthus x giganteus*
2) Degradation of diesel pollution in soil by *Miscanthus x giganteus*

References

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Study of biological effects of new types of carbosilane dendrimers

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Rapidly developing concept of gene therapy brings great expectations in potential treatment of several fatal genetic-based diseases, such as cystic fibrosis, or 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 into 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, a group of nearly monodispersed, highly symmetric, periodically branched polymeric nanoparticles with a near-spherical shape at higher so-called generations (G), have been systematically studied over the past decade as gene delivery vectors due to their attractive properties rivalling the other types of commonly studied polymers. Due to the precisely controlled composition of their core and shell and wealth of surface modification strategies available they possess high potential to surpass many other non-viral vectors in gene delivery applications.

Heretofore, we have synthetized and characterized novel types of carbosilane dendrimers with various types of periphery groups. Also we tested the possibilities of their influence of interaction and effectivity (generation, surface modification) with selected nucleic acids, especially in model cell cultures [2, 3, 4]. Based on obtained results we can summarize that the selected carbosilane dendrimers show low toxicity, relatively high efficiency, and so they could be used as non-viral vectors in targeted drug and/or therapeutic nucleic acids delivery.

Research highlights

1) Phosphonium carbosilane dendrimers were characterized for subsequent use in biomedical applications
2) Carbosilane glucose glycodendrimers are promising efficient vectors in targeted drug delivery
3) Phosphonium carbosilane dendrimers have been shown to be effective, low-toxic non-viral vectors for siRNA cell delivery

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Direct lithiation-halogenation of metallacarborane cluster

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Our work deals with the preparation, isolation and structural characterization of regioselectively B-substituted halogenderivatives of cobalt(III) bis-dicarbollide cluster in order to increase the hydrophobicity, and the antimicrobial activity of the parent molecule. The complex cobalt bis-dicarbolide anion excels in low mammalian cell toxicity, selective antibiofilm, antimicrobial and virostatic activity (HIV-1), significant stability in basic and strongly acidic environments, and is uniquely resistant to UV and gamma radiation. [1-5] The structure and purity of the prepared compounds were verified by available analytical techniques: TLC, HPLC-UV-VIS, MS, NMR, Raman, FTIR ATR, XRD, XRF and the like. In total, four new derivatives were prepared and characterized. The prepared derivatives will be deposited by strong covalent bonds to PES and PAM textiles. The resulting materials will be tested in the next phase by physical-chemical methods and for their catalytic and antibiofilm activity.

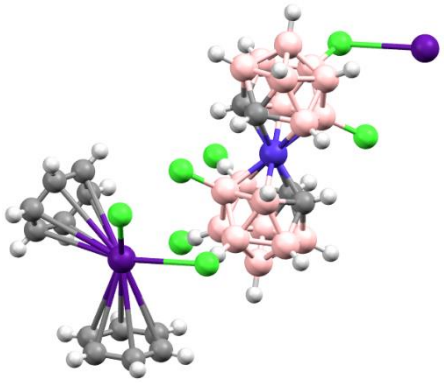

Figure 1: Structure of 4-times chlorinated Cobalt bis-dikarbolide from XRD.

Research highlights:

1. ^{13}C NMR evidence of perlithiation of C-H groups of the cluster.
2. Regiospecific B-halogenation in basic conditions.
3. Optimalization of HPLC-MS method for analytical separation of positional isomers.

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Sulphur particles immobilized on activated polymer surface

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Antimicrobial materials with immobilized or entrapped sulphur particles are of considerable interest. Sulphur as one of the abundant elements on earth is cheap and environmentally friendly. Sulphur nanoparticles can be used as an effective, non-toxic and low-cost alternative to metal nanoparticles [1].

In this work, we have studied the surface properties of polyethylene terephtalate (PET) and polystyrene (PS) foils and changes in its surface properties after activation by ultraviolet radiation and subsequent grafting with sulphur particles (SPs). SPs have been prepared by an acid catalysed precipitation of sodium thiosulphate in the presence of chitosan or sodium dodecyl sulfate as capping agents.

The changes in surface properties of modified foils were characterized by contact angle measurement, electrokinetic analysis and X-ray photoelectron spectroscopy (XPS). The surface morphology of samples and particle sizes were examined by scanning electron microscopy (SEM). The antibacterial activity of the PET samples was tested against *Staphylococcus epidermidis* and *Escherichia coli* bacteria strains. This new nanocomposite has potential to be used in medical applications as antibacterial agent or in food processing as antimicrobial food packaging material.

Research highlights

1) Polymer surface was efficiently activated by UV radiation
2) Preparation of sulphur particles was optimized to achieve desired particle size and narrow size distribution
3) Used analytical methods demonstrated successful grafting of sulphur particles on polymer surface
4) New nanocomposite embodied antibacterial behaviour against tested bacterial strains

Acknowledgement

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Class II biocompatible E-shell 300 3D printing material causes severe developmental toxicity in Danio rerio embryos - implications for 3D printed microfluidics

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Additive manufacturing is a new technology that represents a very promising, cheap and efficient solution for the production of various tools in the biomedicine field. Because of its transparency, user-adjustable properties and high print resolution, photopolymers are steadily increasing in popularity in the area of microfluidics as well. In our study, the toxicity of the commercially available E-shell 300 Series photopolymer, which is used in the manufacture of hearing aids and other implants and which could be potentially exploited in fabrication of microfluidic devices, was tested using in vivo and in vitro biological models.

We examined toxic effect on danio rerio in direct contact with the 3D printed material as well as in water extracts to evaluate the developmental toxicity in vivo. Tests were performed using an OECD standardized Fish Embryo Acute Toxicity (FET) test on Danio rerio embryos. Despite being declared as class-IIa biocompatible, in case of direct contact the results show considerable negative impact embryo development. In this study up to 79 % mortality of in vivo models were observed. Contrary, negligible toxic influence of E-shell 300 water extracts was observed. Further, four different post-processing treatments to reduce this toxicity were tested. We observed that postprinting treatment of 3D printed material in 96 % ethanol can reduce the embryonic mortality in FET test by 71 %.

In summary, our results indicate the importance of biocompatibility testing of the 3D printing photopolymer material in direct contact with the given biological model. On the other hand, the possibility to eliminate toxic effects by proper post-processing strategy opens the doors for broader applications of E-shell 300 photopolymer in the development of complex microfluidic devices for various biological applications.

Research Highlights:
1) An embryonic developmental toxicity of the polymer used in medicine was observed
2) We confirmed the inadequacy of polymer testing based on extracts
3) Post-processing treatments reduce mortality by up 71%

Microfluidic fish embryo test chip with the ability to remove individual eggs during long-term cultivation

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Fish embryo test (FET) is a widely used method for determination of biological activity of substances in vivo. Its popularity comes from the fact that testing on aquatic organisms in general brings advantages in form of lesser costs, easier breeding of the animals and also easier execution of the test itself compared to common tests on mammals, such as rodents. In comparison with invertebrates, fishes have better biological similarity to humans.

New approach in the last years, which is connected with the quick development of lab-on-chip (LOC) devices, brings high potential for improvement of the standard (static) fish embryo test. Our DLP (digital light projection) 3D printed microfluidic chip offers better observing options (higher data efficiency) than in standard FET, more stable, reproducible and overall better cultivation conditions due to continuous medium perfusion and brings potential for automation of many steps of the test. It also addresses the issue of previously developed fish embryo test chips, which were not able to remove the embryos from the device during long-term cultivation. Such option is needed, as it has been proven that dead embryos can have negative impact on other, still living embryos, by releasing harmful substances and/or causing growth of microorganisms. Our chip is capable of removing any individual selected embryo, without affecting the long-term cultivation of other embryos in the system.

Research highlights

1) CFD (computational fluid dynamics) simulations were used to predict the behavior of liquids in microchannels
2) CAD (computer aided design) software and DLP (digital light projection) 3D printing method were used to develop biocompatible microfluidic chip
3) 3D printed microfluidic chip was succesfully tested for long-term cultivation of fish embryos (Danio rerio)

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Plasma treatment of poppy seeds in fluidized bed reactor

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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 coat. 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 150 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 %) six days after planting. Highest rate had samples treated in discharge of power 150 W (85 %). Decrease of water contact angle on treated poppy seeds was observed from 85° (untreated) to 19 – 35° (treated). X-ray photoelectron spectroscopy (XPS) was used to investigate chemical changes on the seeds surface. Untreated sample and 150W treated sample were selected and the chemical state of the surface was observed. Treated sample had slightly increased oxygen and nitrogen content and decreased carbon content on the surface. More significant changes are on C 1s peak and his boundary composition.

Research highlights

1) Plasma treatment has positive effect on poppy seeds
2) Treated poppy seeds had up to 10 % better germination rate than untreated
3) Treated poppy seeds chemical state of surface was changed and that´s the reason why wettability of surface was increased
4) Plasma treatment of seeds in fluidized bed reactor is innovative way, how to improve seed properties

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Application of drones for tropospheric quality monitoring

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Main tasks of this research topic is development of lightweight and power-efficient analytical device capable of real time online measurements of various atmospheric parameters (temperature, humidity, pressure, dust and aerosoles, concentration of several inorganic gases, organic gases, ...) as well as adsorption of volatile organic compounds for ex situ identification and quantitation by gas chromatography coupled to high resolution qTOF mass spectrometer or FID.

Application range for this analytical approach is wide considering extensive atmospheric pollution and significance of various anthropogenic and natural volatile organic compounds (VOCs). It enables correlation of many parameters linked to spatial distribution, therefore versatile and comprehensive atmospheric research.

Table 1 Some of the implemented online sensors and their selected parameters

Environmental parameter	Operating principle	Operating range	Measurement errors	Scan rate	Resolution	Power consumption
Humidity	Polymer capacitor	5 – 99,9 % Rh	3 % Rh	0,5 Hz	0,1 % Rh	250 µA
Temperature	Semiconducting Si diodes	-40 - 80 °C	0,3 °C	0,5 Hz	0,1 °C	250 µA
Atmospheric pressure	Piezoresistive, temperature compensated	0 – 250 kPa	1 %	Up to 100 Hz **	0.1 kPa	10 mA
Dust and aerosole	Light scattering	0,35 – 12,4 µm	5 %	0,03 – 1 Hz	PM 1; 2,5; 4,25; 10 µm	95 mA
VOC	Photoionization detector (Krypton, 10.6 eV)	1 ppbv to 50 ppmv *	2 %	Up to 100 Hz **	10 ppbv	80 mA
NO2	Electrochemical	10 ppbv – 4 ppmv	2 %	Up to 100 Hz **	10 ppbv	90 mA
SO2	Electrochemical	10 ppbv – 4 ppmv	3 %	Up to 100 Hz **	10 ppbv	90 mA
O3 + NO2	Electrochemical	10 ppbv – 4 ppmv	2 %	Up to 100 Hz **	10 ppbv	90 mA
Air mass flow for sorption tubes	Hot-wire	0 – 2 sdm^3/min ***	5 %	2 Hz	50 scm^3/min ***	125 mA
Spatial orientation	GNSS	X, Y, Z axes	Signal and environment dependent (~ 3 m)	0,2 Hz	0.00001°	160 mA

* Isobutylene equivalent ** A/D converter setup dependent *** standard cubic centimeter / decimeter (0 °C, 101.325 kPa)

Research highlights

1) A prototype of analytical device with various sensors and capture of VOCs have been developed.
2) Hardware and software setup is being optimized as well as data treatment and quality assurance.
3) Acquired datasets will be compared to reference measurements (by Czech Hydrometeorological Institute) followed by monitoring locations with known primary pollution.
4) Developed device will contribute to research of atmospheric pollutants and study of natural VOCs
5) Atmospheric research focused on distribution of polutants and study of natural VOCs

Nanofibrous and nanostructured materials for biomedical microfluidic devices

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As current drug testing methods are related to both technical and ethical difficulties, ever growing demand on more rapid and effective drug evaluating process comes with need of different approach. Functional tissue models or whole organs-on-chips seem as promising alternatives to currently widely used animal models.

The key aspect of creating mentioned substitutes lies in specific cell cultivations taking place in precisely controlled microenvironment. That can be achieved by nanostructured surfaces, which enhance the cell cultivations, placed in human body-like conditions prepared via microfluidic devices. Namely the development of so-called tissue barriers is of great importance, because they represent a place where drugs and active agents pass through endothelium from a bloodstream into the tissues. Mimicking the tissue barriers is crucial for advancement in the tissue models and improved drug testing. Therefore, it is one of the main goals of my dissertation.

So far, we have tested possibilities of combining polymeric 3D printed structures and nanofibrous materials to build a novel cell culture model. A polymeric platform was 3D printed from photosensitive resin E-Shell 300 via stereolithography and nanofibers combining modified chitosan, gelatine and polyethylene oxide were electrospun straight onto its surface. During biocompatibility trials, we have discovered strong negative influence of the E-shell 300 on B14 mammalian cells' proliferation. We have successfully negated toxicity of the photopolymer by post-printing treatment of 3D printed materials in ethanol.

Research highlights

1) Progress in novel approach to creating organs-on-chips was achieved.
2) Microfluidic chip combining stereolithography and electrospinning was designed.
3) Nanofibers were electrospun straight onto 3D printed base.
4) Successful cell proliferation after solving toxicity of the photopolymer.

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Specific structure, morphology, and properties of polyacrylonitrile (PAN) membranes prepared by needleless electrospinning; Forming hollow fibers

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Polyacrylonitrile (PAN) membranes have been prepared using needleless electrospinning with wire electrode and characterized by a series of methods HRSEM, XRD, air permeability and area weight measurements in dependence of high voltage and electrode distance. HRSEM analysis revealed the tendency to longitudinal rolling of strip-shaped PAN fibers forming hollow fibers. Combination of XRD analysis and molecular modeling explains this phenomenon as the consequence of the specific crystal structure of PAN fibers, where the isotactic PAN chains are arranged in layers forming belt shaped nanofibers with the strong tendency to roll up longitudinally forming hollow fibers. This effect offers the possibility to create hollow nanofibers by electrospinning with the appropriate choice of structure of polymer chains.

Research highlights:

1) Polyacrylonitrile nanofibers were successfully prepared by needleless electrospinning.
2) Structure and morphology of nanofibers was determined.
3) Important relationship between structure and morphology was found.
4) This method led to simple hollow fiber formation.

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New equipment constructed for bathymetry mapping at the Faculty of the Environment

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Reservoir sediments are a unique source of information about history of the anthropogenic activity in the reservoir catchments. The reservoirs are trap of the sediments, which can also contain the contaminants. The known case is mercury contamination in the Skalka Reservoir [1]. The sediments in the shallow parts of the reservoirs have dynamic evolution and temporal change in volume [2], but sampling is a challenge in contrast to sampling in the central parts of the reservoirs, were is possible to use standard method and equipment. For this reason, new sampling equipment and technics have been developed at Faculty of the Environment (UJEP) [2].

Bathymetric maps (maps of water depth) are needed for rational sediment sampling. The inflatable boat with electric motor is used for the bathymetry mapping at the Faculty of the Environment. This boat has several limits. First is draft of the boat (distance between water level and bottom of the boat), second is low speed and third is uneven data collection.

The first limit was overcome by constructing a light platform attached on the two paddleboards. This platform can be driven by paddles or an electric motor. It allows mapping in shallow parts of the dam in their inflows. Bonus of the system is more comfortable and safer sediment sampling than using of the inflatable boat.

Because shallow parts of the bottoms (inflow deltas) are most dynamic, they require dense bathymetric bottom imaging. It is made possible by our new developed autonomous sonar RC boat. This equipment was developed like catamaran with navigation system ArduPilot [3], a free and open navigation system, which allows plan a boat trip in regular lines. It allows faster and more regular data collection. This RC boat allows take advantage of sonar speed limit which is 15 km/h (the inflatable boat has a max. speed of 5 km/h) that result in considerable shortening of work and/or denser datasets.

Figure 1 Left: Paddleboard platform, Right: autonomous sonar RC boat

Research highlights

1) The floating platform was constructed for shallow water mapping and sampling
2) The autonomous RC boat was constructed for faster and more regular bathymetry mapping

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Room-temperature synthesis of nanoceria for degradation of organophosphate pesticides and its regeneration and reuse

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CeO_2 nanoparticles can be prepared by various procedures, such as calcination of the suitable precursor, reflux or hydrothermal synthesis in an autoclave at elevated pressure, by low-temperature synthesis at 90 °C or using photochemical synthesis. These procedures were compared for preparation of CeO_2 [1,2]. Many studies are focused on the shape engineering of ceria to obtain cubic, rod-like and plate-like [3] particles. However, the calcination at high temperatures or high-pressure treatment or multi-step approach is usually necessary. Modern green chemistry favours low-temperature one-pot syntheses, especially for potential industrial production, where the energy consumption and the complexity of the synthesis and hence its price must be reduced, nevertheless the effect of reaction temperature and the effect of cerium salt concentration was not discussed in detail.

The catalytic activity can be inhibited by the degradation product that leads to inactivation of the catalyst for further use. It is therefore highly desirable to find a way how to prevent or eliminate catalyst inactivation and find an easy process how to regenerate its function. It was suggested that -OH surface groups are consumed during the degradation reactions but can be easily replenished and thus the catalyst can be regenerated.

In this work [4], we prepared nanocrystalline cerium oxides by simple low-temperature synthesis. We demonstrated that by simple changing of the reaction temperature, the properties such as particle size, specific surface area, porosity or surface chemical composition can be modified. The catalytic activity of prepared materials was tested by decontamination of parathion methyl in non-aqueous solution. Reusing of catalyst led to the decrease of its catalytic activity although this was not observed during testing in water in our previous study [5]. We combined these two procedures and demonstrated that the catalyst used in a non-aqueous solution can be reactivated by water washing for further use.

Research highlights

1) Uniform CeO2 nanoparticles were prepared under ambient conditions in water
2) Particle size from 5 to 15 nm can be controlled by the synthesis temperature
3) The amount of oxygen vacancies significantly affects the degradation activity
4) Catalyst reactivation can be achieved by simple water washing

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Seasonal accumulation of manganese content in three plant species of forest ecosystem affected by anthropogenic activities

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Essential function of Mn in plants is well known. Normal Mn concentrations in plant dry matter are 20 – 500 mg kg^{-1}. Some plants can accumulate excessive levels of manganese without showing any toxicity symptoms. Such plants are called hyper-accumulators. They can accumulate over 10000 mg $kg^{-1}$of Mn in dry mass [1]. The limit of toxicity, as well as tolerance to excess of this metal, is dependent on the plant species [2]. Its availability for plants is favoured in acidic soils [3]. The Mn phytotoxicity is a nutritional disorder that is often not clearly identified. In turn, it can be the result of complex interactions with other elements (K, Ca, Fe, Si) and some habitat conditions [4].

The presented contribution is based on a survey (2010 – 2019) of manganese accumulation in assimilation organs of selected forest plant species in an area highly affected by anthropogenic activities connected mainly with coal industry (North Bohemian Basin) with proven elevated levels of Mn in soil (Ah – 1613 mg kg^{-1}, B – 3165 mg kg^{-1}, pH 3.86 – 4.14). Three forest species have been selected for the long-term observation so far (bilberry - *Vaccinium myrtillus* L., european larch - *Larix decidua* Mill., silver birch - *Betula pendula* Roth.). All of them showed Mn accumulation in leaves during the growing seasons (May – October) in 2010 – 2019 with maximum values exceeding 10000 mg kg^{-1}, and also significant dependence on cumulative rainfall. To prove our hypothesis that acidification of soils, through acid deposition from sources of pollution, in combination with high values of Mn in soils and rock environment with low buffering capacity, further monitoring of manganese in soils and in bilberry leaves in larger area of eastern Ore Mountains was executed. The normalization of the comprehensive dataset with calcium concentrations in the soil horizons Ah and B, due to the antagonistic relationship with Mn, so far confirms the hypothesis, but additional analyses need to be made concerning Ca levels in monitored plant foliage.

Research highlights

1) Long-term monitoring of manganese accumulation in forest ecosystem was performed.
2) Levels of Mn exceeds hyper-accumulation limit in leaves of selected plant species.
3) Mn content in leaves of bilberry, larch and birch depended on cumulative rainfall.
4) Mn accumulation assigned to soil acidification and rock environment.

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