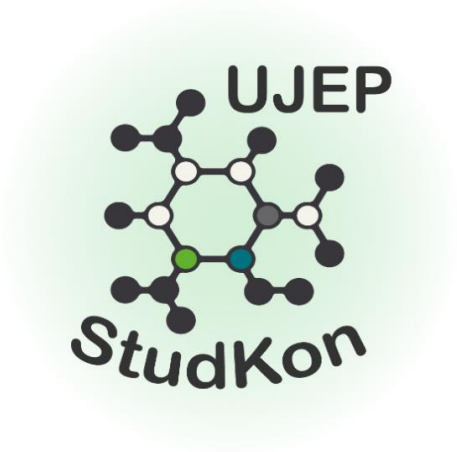
JAN EVANGELISTA PURKYNĚ UNIVERSITY IN ÚSTÍ NAD LABEM
Faculty of Environment

JAN EVANGELISTA PURKYNĚ UNIVERSITY IN ÚSTÍ NAD LABEM
Faculty of Science



BOOK OF ABSTRACTS

6th Conference of Natural Sciences and Technical PhD study programmes at UJEP

StudKon 2023

26. 6. 2023

Centre of Natural and Technical Sciences

J. E. Purkyně University in Ústí nad Labem

http://www.studkon.ujep.cz

StudKon 2023 programme:

MONDAY 26. 6. 2023	
Registration	**8 – 9 a.m.**
Morning sessions	**9 a.m. – 1:50 p.m.**
9:00 – 9:20 a.m.	Opening and welcome session, introduction of guests
9:20 – 10:40 a.m.	**Talks session 1** 9:20 Štěpanovská Eva 9:40 Syrový Michal 10:00 Šulc Martin 10:20 Dušková Tereza
10:40 – 11:10 a.m.	Coffee break
11:10 a.m. – 12:30 p.m.	**Talks session 2** 11:10 Štěpka Jan 11:30 Bílková Gabriela 11:50 Boonen Katrien 12:10 Kwoczynski Zdeňka
12:30 – 1:50 p.m.	Lunch break
Afternoon sessions	**1:50 – 6:00 p.m.**
1:50 – 2:00 p.m.	Jiří Orava: Introduction of UJEP research equipment database
2:00 – 3:20 p.m.	**Talks session 3** 2:00 Harrandt Václav 2:20 Paříková Anna 2:40 Panuška Petr 3:00 Snow Jan
3:20 – 3:30 p.m.	Taking photo together
3:30 – 5:30 p.m.	**Poster session** + secret quiz for the audience + light refreshment
5:30 – 6:00 p.m.	Technical break
Evening programme	**6:00 – 10:00 p.m.**
6:00 – 6:30 p.m.	Feedback to students (presentation skills and scientific content)
6:30 – 7:00 p.m.	The Miroslav Broul award ceremony
7:00 – 10:00 p.m.	Barbecue

List of participating PhD students and their contributions:

Talk session 1

- **Štěpanovská Eva** (PřF): Modification of graphene oxide and polymer films with energetic ion beams for their use in lithium battery applications
- **Syrový Michal** (PřF): Simple one-step preparation of functional nanofibrous materials for CO_2 capture
- **Šulc Martin** (FŽP): Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral
- **Dušková Tereza** (PřF): Metal complexes with polyfluorinated NHCS

Talk session 2

- **Štěpka Jan** (PřF): Analysis of the effect of CeO_2 nanoparticles on microbial communities in anaerobic digestion process of biogas plant
- **Bílková Gabriela** (FŽP): Factors controlling Mn contents in leaves of silver and downy birch in acid soils of central Europe and Norway
- **Boonen Katrien** (FŽP): Which factors influence mercury accumulation in tree rings?
- **Kwoczynski Zdenka** (FŽP): Biochar from local biomass waste as a soil amendment - The effect on the bioavailability of elements

Talk session 3

- **Harrandt Václav** (PřF): The electrodiffusional theory for wall shear stress measurement by two-strip probe: a journey to near-wall region hydrodynamics
- **Paříková Anna** (PřF): Condensational growth of submicrometer particles for targeted high-efficiency pulmonary delivery
- **Panuška Petr** (PřF): A microfluidic chip for generation and cultivation of tumor spheroids fabricated from OSTE+ polymer.
- **Snow Jan** (FŽP): Removal of chlorine during pyrolysis of plastic waste

Poster session

- **Aubrecht Petr** (PřF): non-public title and abstract
- **Dědičová Šárka** (PřF): Effects of external electric fields on the structure of oligo(ethylene glycol) in explicit solvents by molecular dynamics simulations
- **Fales Alexandr** (FSI): Educational robotics
- **Greguš Viktor** (PřF): Association of cobaltacarborane derivative in aqueous solutions: Light scattering study
- **Hamalová Kateřina** (PřF): Amine-doped PEBA membrane for CO_2 capture
- **Hoskovec Jakub** (PřF): Polyurethane nanofiber membranes modified by amines for CO_2 capture
- **Kocholatá Michaela** (PřF): Isolation and characterization of plant exosomes for biomedical applications

- **Mamirova Aigerim** (FŽP): Biochar-driven phytoremediation of complex contaminated sediments: Case study of Paulwonia tomentosa
- **Matysová Pavlína** (PřF): Molecular simulations of salts hydrates
- **Newton Robert Ato** (FŽP): Impact of soil amendments on the production of Miscanthus × giganteus biomass at the slightly contaminated post-mining areas
- **Poustka David** (PřF): Straight channel microfluidics for viscoelastic exosome separation – Influence of geometry and materials
- **Vaněk Martin** (FŽP): Determination of Mercurialis ovata and Mercurialis perennis hybrids according to morphological features and genome size

Talks session 1
(9:20 – 10:40 a.m.)

Modification of graphene oxide and polymer films with energetic ion beams for their use in lithium battery applications

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[b]*Institute of Nuclear Physics of CAS, v.v.i. Husinec-Rez, 250 68 Rez, Czech Republic*

**Eva Štěpanovská, email: stepanovska@ujf.cas.cz, 2nd year of PhD, Applied Ion Technology*

This work focuses on the implantation of Li, Cu, and Ag ions into graphene oxide (GO), polyimide (PI), polymethyl methacrylate (PMMA), and cyclic olefin copolymer (COC) thin films. The energy of the implanted ions ranges from 150 keV to 45 MeV, depending on the need to modify the surface or the entire volume of the material. The ions were implanted at different ion fluences [1×10^{12}, 1×10^{14}, 1×10^{16}] cm^{-2}. The aim of modifying these organic materials is to increase the carbon concentration, reduce the concentration of oxygen and hydrogen-containing functional groups, and simultaneously implant Cu and Ag ions into the internal structures of these materials. Changes in the elemental composition will be monitored using RBS/ERDA, changes in chemical bonds using XPS, Raman spectroscopy, and FTIR, and changes in morphology using SEM and AFM. Additionally, measurements of the electrical properties of the materials, specifically electrical conductivity, capacity, and coulombic conductivity, will be conducted. The purpose of implanting organic materials is to test them as suitable anode and electrolytic materials for lithium batteries (LIB). The modification of materials and their assembly into a functional battery is carried out in cooperation with the Helmholtz-Zentrum Dresden Rossendorf (HZDR) and the University of Chemistry and Technology, Prague (UCT).

Simple One-Step Preparation of Functional Nanofibrous Materials for CO_2 Capture

Michal Syrový[a,*], Pavla Čapková[a], Petr Ryšánek[a], Monika Vostiňáková[a], Kateřina Hamalová[a], Daniel Bůžek[b], Oldřich Benada[a,c]

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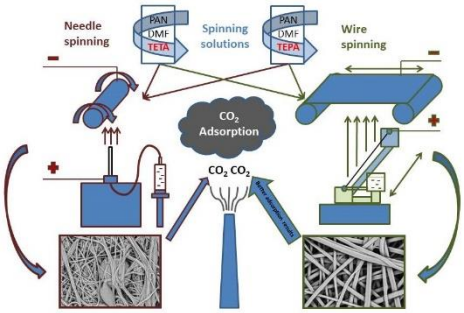
Nanofibrous materials prepared by electrospinning provide a wide range of applications from biomedical applications to filtration and separation media to catalytic membranes. A key problem in the preparation of nanofiber materials for specific functions is the chemical modification of nanofiber surfaces. In this work, I focus on electrospun polymer (polyacrylonitrile (PAN), cellulose acetate (CA)) nanofibrous membranes modified with different types of amines (different number of amine functional groups) and Zr-based metal organic frameworks for CO_2 capture. Electrospinning technology can be used in different variations and in this case I will deal with two main technologies for the preparation of 2D nanofibrous membranes: needle spinning and wire spinning. It turns out that the arrangement of the spinning device has a significant effect on the structure, properties and functionality of the membranes.

As a part of work, I also discuss two approaches to the chemical modification of nanofibrous surfaces: (1) one-step technology, i.e. adding a modifying substance directly into the polymer solution and (2) postspinning modification - subsequent deposition of the modifying substance on the nanofibrous membrane. The effect of all these technological variations is demonstrated on sorption capacity of membranes based on polyacrylonitrile and cellulose acetate modified with amines and MOFs. [1-4]



Research highlights

1) Easy, fast and low cost preparation of reusable functional material for CO_2 capture.
2) Wire spinning technology seems more suitable for adsorption due to higher permeability of textiles.
3) Pure cellulose acetate, as a more bio-friendly material, shows similar CO_2 capture as amine-modified polyacrylonitrile.

References

[1] Syrový M., "Effect of electrospinning parameters on the structure and morphology of PAN - based nanofiber membranes," Jan Evangelista Purkyne University – bachelor thesis (written in czech), 2019.

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[4] Syrový M., et al. "Effect of wire and needle spinning on the direct manufacturing PAN/amine nanofibrous membranes for CO_2 sorption", **DOI:** 10.1177/15280837231176083 (accepted article)

Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral

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The Czech Republic has significant reserves of lithium in the form of mica in the mineral zinnwaldite. The total reserves of ores with increased lithium content at Cínovec were estimated to have least 300 Mt with an average metal content of 0.117% Li. [1]

Several technologies of zinnwaldite concentrate processing have been in the years 1953 to 1967 developed at the Research Institute of Inorganic Chemistry in Ústí nad Labem. The best yield was shown by the gypsum method based on thermal sintering of the concentrate with a $CaSO_4$ and $Ca(OH)_2$. For all the technology tests done in the past only alkaline additives of laboratory purity were used.

The aim of my research is to modify the original laboratory gypsum method for the use of real additives - technical calcium hydroxide and natural gypsum or energy gypsum. Today is only one active mine for natural gypsum in Kobeřice near Opava in the Czech Republic. This represents a long transport distance of the raw material of 450 km. Therefore, it would be appropriate to replace natural gypsum from lalternative sources. Because Zinnwaldite deposits are located in Northern Bohemia, where Since most of coal-fired power plants in Czech Republic are located it's our best option to try use energy gypsum. As we know during the desulphurization of their flue gases, a practically unlimited amount of energy gypsum is produced, which is sold cheap as certified raw material.

Was comparated the chemical composition of energy gypsum samples from fift different coal-fired power plants and two natural gypsum samples from Czech republic and Poland. As the most suitable was energy gypsum from power plant Ledvice and natural gypsum from Kobeřice yet. This materials are using as an alkaline additive in the melting now.

The melting batch consists of zinnwaldite concentrate, gypsum $CaSO_4 . 2H_2O$ and $Ca(OH)_2$ in a ratio of 6 : 4,2 : 2. Three fusion mixtures were created. A - additives of laboratory purity, B - natural gypsum additives, C - energy gypsum additives. All these mixtures were simultaneously melted at temperatures of 850-1000 °C and a residence time in the furnace of 15-90 minutes. The resulting clinkers were ground, dissolved and leached in water. The ideal temperature and leaching time for each mixture is now being evaluated according to the amount of lithium converted to solution. The composition of the obtained sulphate extracts allows their simple and effective purification. Using K_2CO_3 potassium carbonate, it is then possible to precipitate relatively pure Li_2CO_3, which is suitable both for sale and direct use in industry, and for the production of lithium compounds, including high-purity Li_2CO_3. [2]

Research highlights

1) Lithium carbonate
2) Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral
3) Utilization of Zinnwaldite Wastes for Recovery of Lithium
4) Li concentrate from waste raw materials generated during the separation of tin and tungsten

References

[1] Botula, J., Rucký, P., Řepka, V. (2005). Extraction of zinnwaldite from mining and processing wastes.

[2] Jandová, J., Dvořák, P., Vu, Hannah. (2010). Processing of zinnwaldite waste to obtain Li_2CO_3.

Metal Complexes With Polyfluorinated NHCS

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Metal-N-heterocyclic carbene complexes containing three or six fluorous ponytails were prepared. All of these rhodium, ruthenium, and iridium NHC-type organometallic complexes were characterized by HRMS, EA and multinuclear NMR spectroscopy. Fluorophilicity (f) of fluorinated NHC transition metal complexes were determined by their partition coefficients (P) in the standard solvent system (perfluoro)methylcyclohexane/toluene. The Tolman electronic parametr of fluorinated NHC was deteremined by FTIR.

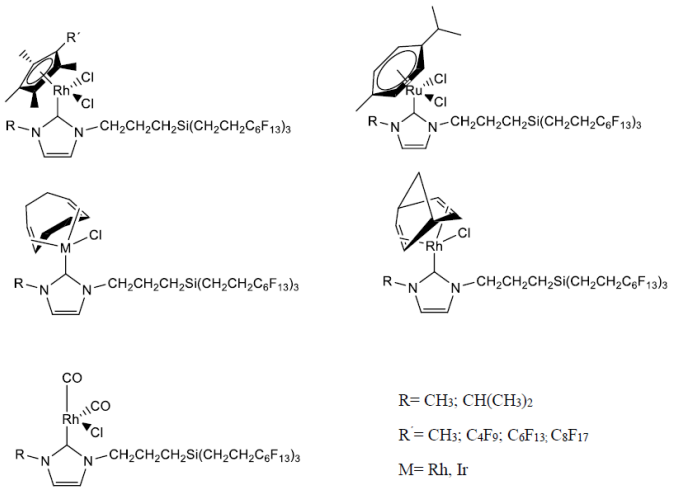

Figure 1 NHC-complexes

Due to the increasing needs of the industry the environmentally friendly synthesis process is an important objective. The use of fluorous compounds in catalysis is well known for highly efficient recycling of catalysts. Therefore, the catalytic activity of ruthenium catalysts was investigated. The catalysts were used in the transfer hydrogenation of cyclohexanone. The adsorption (physisorption) of the fluorous catalysts on a solid fluorous substrate such as fluorous silica was also investigated.[1] Biological activity of such compounds will be also studied, with the focus on study of their possible applications in biomedicine. [2,3]

Research highlights

1) New metal (Ru, Rh, Ir) complexes of NHC ligands bearing polyfluoralkyl tag were prepared.
2) Study of activity of metal complexes in two-phase catalysis system, e.g in transfer hydrogenation was started.

References

[1] Vincent J-M.; Biphasic Chemistry and The Solvent Case; John Wiley & Sons, 2020, doi: 10.1002/9781119695080.ch2.

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[3] Lundgren, R. J., Rankin, M. A., McDonald R., Schatte G., Stradiotto M.; *Angewandte Chem. Int. Ed.*; **2007**, 46, 4732-4735, doi: 10.1002/anie.200700345.

Talks session 2
(11:10 a.m. – 12:30 p.m.)

Analysis of the effect of CeO_2 nanoparticles on microbial communities in anaerobic digestion process of biogas plant

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Due to global production and application of cerium oxide nanoparticles in various industrial sectors, most of the nanomaterial end up in water and soil, where they interact with soil microorganisms and plants. Considering the biogas generation as the final stage of the biochemical conversion of organic matter (under anaerobic conditions to biogas and residual fermented material), the process itself might be affected by the previous nano-pollution. Using organic matter acquired from local biogas plant a cultivation experiment was established to determine nature of the interaction between CeO_2 nanoparticles and the complex anaerobic microbial community. Molecular analysis of the cultivated microbial communities was carried out by an extraction of DNA of each sample, PCR focusing on procaryotic and eukaryotic organisms, MID/Tag marking to differentiate each sample and next-generation DNA sequencing using platform MiSeq-Illumina. Results comprise data of the sensitivity of wide array of microbial taxa.

References

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Factors controlling Mn contents in leaves of silver and downy birch in acid soils of central Europe and Norway

Gabriela Bílková[a*], Tomáš Matys Grygar[a], Michaela Königová[a], Jitka Elznicová[a], Belinda Flem[b]

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The mountain forests in Europe have been damaged by soil acidification that peaked around the mid-20th century. Subsequent spruce forest dieback was most disastrous in the 1970s and 1980s. Before the end of the 20th century the acid emissions were considerably reduced, but forest recovery has been slower than expected. One reason of the delayed recovery could be an excessive bioavailability of Mn in acidified soils that promoted plant species highly tolerant to Mn via its accumulation and internal sequestration, such as birch. The aim of our work was to examine factors governing elevated Mn uptake by birch, which is apparently the feedback mechanism keeping the Mn bioavailability high even after mitigation of acid rains.

Our research combines own collections as well as analysis of data from literature. In 2022, we sampled silver birch (*Betula pendula*) leaves in Czech Republic, along Czech state borders, and in the Harz Mts. and Thüringer Wald Mts., Germany. Laboratory element analysis was performed with energy dispersive X-ray fluorescence spectrometry (XRF). Literature data concerned downy birch (*Betula pubescens*) collections from Norway, published by the team of influential environmental geochemists Clemens Reimann.

Foliar concentrations of Mn in birch trees result from an interplay of geological, geochemical, pedogenic, topographic and anthropogenic controlling factors. Foliar Mn concentration is elevated in case of low macronutrient uptake (Mg, sometimes also K), in soils on felsic or silicic rocks (they are nutrient poor, or nutrients are only slowly liberated due to slow rock weathering), and soils impacted by acid rains and metallurgy emissions [1]. High Mn accompanied by high Zn in birch leaves could be a diagnostic tool to map the consequences of soil acidification and contamination from metallurgy. The Mn concentration in several subsets were controlled by altitude and/or topography of the sampling sites. All conclusions obtained for our central European collections of silver birch were supported by evaluation of downy birch datasets from Norway. Distribution of Mn in leaves was studied by XRF scanner at the University of Turku. Birch trees with high Mn concentration have a different strategy of Mn sequestration in leaves. The Mn and Zn content in birch leaves appears to be suitable for geochemical mapping of consequences of historical soil acidification and contamination.

Research highlights

1) Birch leaves for mapping soil acidification and metallurgy contamination
2) Upgrade of previous work on Mn in birch leaves to European level
3) Identification of two types of Mn acquisition strategies of birch

References

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Which factors influence mercury accumulation in tree rings?

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Trees could be used as an archive of environmental pollution in regions where pollution monitoring has not, or only recently, been implemented and no geochemical archives are available. Mercury (Hg) is a promising trace metal for the reconstruction of historical air pollution, since its primary uptake pathway was found to be from the air by the leaves, from where it is transported through the phloem to the tree rings [1]. Although several authors have found that tree-ring Hg concentrations reflect atmospheric exposure concentrations [2, 3], this was not the case for all studies on this topic. One of the reasons for the lack of consensus is that the factors that influence the Hg concentration in tree rings are not yet well understood. This research aims to identify factors other than the Hg concentration in the air, such as the tree growth rate, climatic variables and tree species, that influence the Hg concentration in tree rings.

Cores of five species (*Larix decidua*, *Pseudotsuga menziesii*, *Robinia pseudoacacia*, *Acer platanoides* and *Prunus avium/cerasus*) were sampled in Ústí nad Labem. After measuring and dating the tree rings, the cores were cut into separate annual rings and freeze-dried. Hg in each ring was measured with a cold vapour atomic absorption (CV-AAS) Hg analyser. Historical air pollution data were obtained from the Czech Hydrometeorological Institute [4]. Linear mixed models suggest that tree-ring Hg is also influenced by factors other than Hg in air. In larch, tree-ring width was found to be the factor with the highest correlation with tree-ring Hg concentration. This seems to be partially due to a coincidental match between peak growth and peak air pollution in the 1980s. An additional explanation could be that higher stomatal conductance in years with good growth conditions (especially enough summer precipitation) results in photosynthesis products with more Hg bound to them. In other species, tree-ring water content showed a significant correlation with tree-ring Hg. This knowledge of the factors that influence Hg concentration in tree rings can help to compose models for reconstructing historical atmospheric Hg.

Research highlights

1) Hg in tree rings is influenced by factors other than atmospheric Hg.
2) Tree-ring Hg concentration and its temporal trend differ among species.
3) Tree growth appears to affect the Hg concentration in rings of larch.

References

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[4] Atmospheric Hg^0 measurements from ISKO database, CHMI, and Hg emissions Spolchemie from REZZO 1 database, CHMI.

Biochar from local biomass waste as a soil amendment - The effect on the bioavailability of elements

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The production of biochar by pyrolysis of biomass waste represents a cleaner and more sustainable treatment compared to direct combustion [1]. Moreover, produced biochar can be further variously utilized. Used as soil amendment, biochar can improve soil properties in many ways. Biochar supports microbial growth in soils [2]. The addition of biochar to the soil also causes aeration [3] and increases the soil's ability to retain moisture and thus the nutrients that are dissolved in [4]. It is a way of biological sequestration of carbon [5]. The use of this type of fertilizer will also reduce the need for industrially produced fertilizers [6].

Depending on the selected raw biomass and pyrolysis condition, the composition and properties of the produced biochar change [7]. Before the pyrolysis itself, a comprehensive characterization of the local biowaste was carried out. The pyrolysis conditions were optimized and the produced biochars were analyzed. After evaluating all the obtained results, due to its properties and elemental content the sample Extracted rapeseed meal was chosen as the most suitable waste biomass suitable for the production of biochar applicable as a soil amendment.

To verify the positive effect of the addition of biochar, a pot experiment was carried out on lettuce (*Lactuca sativa L.*), which grew in the soil for two growing seasons. In this experiment, the effect of biochar addition on biomass yield, soil properties and especially on the elemental composition of soil and biomass were evaluated. Emphasis was placed on determining the bioavailable fraction of elements by Mehlich 3 soil extraction, which most authors neglect to analyze. Although this analysis provides very valuable information about a more realistic soil nutrient content, since plants receive elements only in certain forms. An increase in the total concentration of a nutrient in the soil does not equal an increase in the concentration available to plants. Based on the obtained results, it can be summarized that the addition of biochar to the soil significantly increases the concentration of nitrogen, potassium and phosphorus, but only in the case of potassium, the bioavailable fraction also increased. This increase of nutrients corresponds to a higher biomass yield after the addition of biochar.

Research highlights

1) Extracted rapeseed meal was evaluated as a most suitable raw material
2) The addition of biochar improves soil properties and increases biomass yield
3) Addition of biochar cause a significant increase of bioavailable forms of K

References

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Talks session 3
(2:00 – 3:20 p.m.)

The electrodiffusional theory for wall shear stress measurement by two-strip probe: a journey to near-wall region hydrodynamics

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**Presenting author, e-mail: vaclavharrandt@seznam.cz 1st year of PhD, Computer Modelling in Science and Technology*

Transport phenomena occurring in the near-wall region depend on the hydrodynamics in the boundary layers and are, therefore, significantly influenced by the behavior of the wall shear stress [1]. For this reason, the knowledge of the velocity gradient in the immediate vicinity to the solid surface can be used to optimize problems concerning fluid dynamics, such as, for example, the reduction of the drag coefficient of vehicles, the intensification of chemical processes in the industry, or for findings of adequate conditions during the cultivation of biological material in biotechnological applications.

One of the possible techniques for non-intrusive measurement of the wall shear stress is the electrodiffusion method developed by Reiss and Hanratty [2,3]. The basic principle lies in measuring the limiting electric current flowing through the electrode flush-mounted with the wall. On the basis of the value of the electric current is subsequently possible to describe hydrodynamics near the wall. Nevertheless, in order to obtain the studied hydrodynamic quantities from the electric current signal, appropriate relations are needed, which can be found by using a theory that analytically describes the investigated problem.

This contribution deals with a new theory [4] describing the mass transport in the vicinity of the measuring two-segment strip probe. Analytical formulas for the mass transfer coefficients of the front and the rear electrodes were derived. The correctness of these formulas was confirmed by the numerical solution of the convection-diffusion transport equation. Furthermore, a methodology for possible experimental data treatment was proposed. From the analysis of the electric current ratio predictions, an optimal probe configuration was found with respect to the sensitivity of the flow direction measurement. Applying the presented derived theory to the experimental measurements makes it possible to determine both a wall shear stress magnitude and its direction.

Research highlights

1) New electrodiffusional theory for a two-strip mass transfer probe is presented.
2) Arbitrary direction of fluid flow over an optional probe geometry is considered.
3) Analytical formulas for the mass transfer coefficient are derived.
4) Methodology for wall shear rate measurements with a two-strip probe is proposed.

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Condensational Growth of Submicrometer Particles for Targeted High-Efficiency Pulmonary Delivery

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More than 300 million of people worldwide suffers by asthma. Not only do half of the patients use conventional inhalers incorrectly but inhalers themselves are also not very efficient at delivering pharmaceutical aerosols to the lungs. A high percentage of the aerosol is deposited in the oral cavity resulting in wasted medication and increased side effects (including cancer). One approach to reducing the deposition in this region and therefore increasing the efficiency of the drug is controlled aerosol growth. This is achieved by introducing dry submicrometer particles of a hygroscopic nature. As they enter the system together with the air at a temperature lower than body temperature, the water vapor present condenses on the particles resulting in the desired growth.

This work presents experiments and basic numerical simulations of an apparatus with a bent tube that corresponds to the human mouth-throat region – the critical area of aerosol deposition. As a hygroscopic substance, sodium chloride was used. The effect of relative humidity and initial particle size on the aerosol growth was studied. The initial particle size was measured using a Scanning Mobility Particle Sizer spectrometer and the grown particles by Aerodynamic Particle Sizer spectrometer. Based on the measured sizes the growth factor was evaluated. Numerical computational fluid dynamics simulations were focused on the description of heat, mass, and momentum transport. Particle motion and growth were performed by applying Newton's second law and the interaction between the flowing fluid and the moving particle was described by the one-way approach.

Research highlights

1) Mouth-throat is crucial for inhaled drugs; standard inhalers are inefficient.
2) Controlled aerosol growth improves drug delivery by reducing oral deposition.
3) An apparatus resembling a respiratory system was set up.
4) Preliminary results show the growth factor of aerosol as expected.
5) Relative humidity does not affect the growth factor.

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A microfluidic chip for generation and cultivation of tumor spheroids fabricated from OSTE+ polymer.

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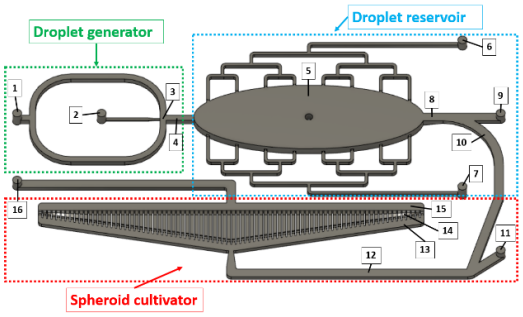
Tumor spheroids offer a more precise method for testing pharmaceuticals compared to conventional 2D cell cultures. Droplet microfluidics is a promising approach for creating uniform spheroids, which requires minimal usage of medium and cells, and enables easy observation of the formation process. However, droplet-based methods have a disadvantage: the cells' limited lifespan in individual droplets due to the difficulty in renewing the medium. To overcome this issue, we are designing a system that can transfer the spheroids from droplets to a continuous water phase and trap them using hydrodynamics. This approach allows for automated medium renewal.

The chip uses the cross-junction droplet generation principle to encapsulate cancer cells in individual droplets, dispersed in hydrofluorether HFE-7500, where they form spheroids. The chip allows for coalescing the droplets into a continuous water phase by flushing the emulsion with a destabilization agent once the spheroids are formed. The released spheroids are then transferred into a cultivation part where they are trapped in separated chambers. The spheroids can be further cultivated in perfusion mode, allowing the testing of various anti-cancer pharmaceuticals. All the steps are performed inside the chip, eliminating the need for external spheroid handling.

Figure 1 Illustration of the inner strucutre of the microfluidic systém.



Research highlights

1) OSTE+ polymer has been successfully tested for manufacturing of complex design, repeatedly-useable microfluidic chip.
2) A droplet-based microfluidic chip capable of long-term cultivation of 3D cell cultures has been developed.

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Removal of chlorine during pyrolysis of plastic waste

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As a complement to mechanical recycling, pyrolysis can be used to recycle complex mixtures of municipal waste plastics (MPW). The subsequent introduction of the liquid product into petrochemical processes can yield virgin polymers. However, there are strict petrochemical limits regarding liquid properties, particularly heteroatom content. In this sense, chlorine is highly inflected because of downstream corrosion and product degradation. The present work, therefore, deals with the possibility of its removal directly in the pyrolysis process. For this purpose, pyrolysis of a model and a real mixture of waste plastics was performed using different temperature programs and dehalogenation agents. The results show a reduced dechlorination efficiency in the pyrolysis of waste plastics, which was subsequently explained by PET and cellulose interactions with HCl that led to the increased formation of more stable chlorinated hydrocarbons. These compounds then pose higher demand on the efficiency of commonly used dechlorination agents. In the present study, we propose a novel mixture of dechlorination agents, which shows a synergistic effect towards dechlorination during MPW pyrolysis based on the interaction of zeolite and hydrotalcite. In combination with stepwise pyrolysis, their presence in a 1:1 ratio decreased Cl content in liquid product from 269 ± 34 pmm to 12,2 ± 1,2 ppm. Considering the use of the product as a minor addition to the current technological streams, the achieved dechlorination efficiency may be sufficient.

Research highlights

1) Dechlorination is hindered in the presence of PET or cellulose.
2) Chlorinated hydrocarbons were found in both products from stepwise pyrolysis.
3) Other heteroatoms (O, S, N, P) were partially removed by stepwise pyrolysis.
4) 95% dechlorination efficiency with β-zeolite and hydrotalcite mixture (1:1)

Poster session
(3:30 – 5:30 p.m.)

Effects of external electric fields on the structure of oligo(ethylene glycol) in explicit solvents by molecular dynamics simulations

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Understanding the structure of polymer solutions under external electric field is very important for applications, such as electrospinning technology [1]. Molecular dynamics simulations were performed under various applied external electric field for oligo(ethylene glycol) of different chain lengths in water or methanol in order to explain the results of our previous study [2]. In a molecular dynamics simulation, we characterize the anisotropy of the average shape of the coil by quantities derived from the gyration tensor. The distribution of the cosine of the angles of the vector of the monomer unit and the dipole moment vector with respect to the electric field direction is calculated. Results show that the coil in both solvents becomes an increasingly anisotropic and adopts oblate average shape with stronger fields, but in water this feature seems to be diminished by increasing chain length. In water, the monomer units of the chain orient at angle of about 70° whereas, in methanol, the monomer units orient perpendicular to the electric field. The monomer dipoles of the chain in both solvents point an increasingly in field direction.

Research highlights

1) Perform molecular dynamics of ethylene glycol oligomers in polar solvents.
2) Identify structural changes of an oligomer molecule induced by an electric field.
3) Describe the effect of the electrostatic field intensity and chain length on studied changes.

Acknowledgements

This research has been supported by the Jan Evangelista Purkyně University in Ústí nad Labem within the student grant programme (Project No. UJEP-SGS-2022-53-002-3). Computational resources were supplied by the project "e-Infrastruktura CZ" (e-INFRA LM2018140) provided within the program Projects of Large Research, Development and Innovations Infrastructures.

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Educational robotics

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This research deals with educational robotics and the use of robotic kits in teaching. One of the goals was to find out which robotic kits are used today for teaching robotics in primary and secondary schools in the Czech Republic. The research took place in the form of personal consultations during training, webinars and project days directly with principals, deputy principals and pedagogues who will apply educational robotics in teaching. A total of 2156 participants took part. At the moment, the platforms of robotic construction kits VEX and LEGO are the most used in primary and secondary schools. VEX in GO versions, IQ gen 1 and gen 2. LEGO in WeDo 2.0, MINDSTORMS EV2 and EV3 and SPIKE versions. Micro:bit and Arduino are also used.

Another goal was to find out the current requirements of educators in the field of educational robotics. The result is a need for training in construction, diagnostics and programming. The main requirement of educators is a methodology for educational robotics for the platform VEX GO and VEX IQ generation 2 using generation 1. I have personally tested all the listed robot kits. Educational robotics using STEM/STEAM/STREAM methods is the most suitable form for teaching robotics with a focus on construction, diagnosis, algorithmization, coding, programming and reviving a real robot. For students, this form of teaching is interesting, beneficial, interactive, fun, purposefully research-based, educational, and above all, it actively involves the student in his or her own self-education process. Validated on 1260 students.

Figure 1 *VEX IQg2 - Clawbot*

Research highlights

1) Robotic kits in primary and secondary schools are mostly from the VEX and LEGO platforms.
2) Educators need training in constructions, diagnostics and programming. They need methodology for VEX.
3) Educational robotics with the STEM/STEAM and STREAM method is the most suitable form for teaching.

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Association of Cobaltacarborane Derivative in Aqueous Solutions: Light Scattering Study

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This work is focusing more closely on the aggregation behaviour of the hydrophobic heteroborane cluster [8-(1,4-dioxane)-1-ium-*closo*-1,2-dicarba-3-cobalta(III)dodecaborane(10)-3-*commo*-3'-*closo*-1′,2′-dicarba-3′-cobalta(III) dodecaborate(11)] (further as C8D) in aqueous solution.

The specific reactivity of C8D enables the possibility of its use as a safe and productive precolumn derivatization agent for the analytical determination of structurally different biogenic amines, monitored products of aminoacids decarboxylation mostly in food and beverages. The very low solubility of C8D in water combined with the optimization assumption of the predominantly aqueous nature of real analyte samples previously proved to be a limiting factor in the quantitative progress of the derivatization reaction, which we had previously put forward as a reagent particle aggregation issue that could only be overcome by long-term sonication in a heated bath. Our aim was to describe the size of the formed particles and the deaggregation efficiency of sonication with help of dynamic light scattering technique. The aggregation behaviour of the derivatization reaction is a rather complex problem also due to the large number of side reactions involved, requiring further study using microscopy and separation techniques, which are planned in the near future.

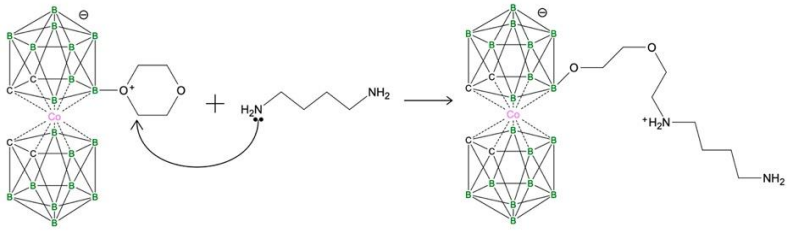

Figure 1 Scheme of the ring opening derivatization reaction of putrescine (Terminal B-H and C-H atoms not shown for clarity)

Research highlights

1) The first DLS study of the de/aggregation behaviour of C8D at specified conditions.

References

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Amine-doped PEBA membrane for CO_2 capture

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In recent years, mixed matrix membranes (MMMs) have been used more often in separation processes due to their excellent properties. These membranes combine the advantages of two main components, the polymer continuous and the nanoparticle dispersion phases [1]. Block copolymers such as poly(ether-block-amide, PEBA) seems to be excellent materials for the membranes synthesis. This work aims to provide an overview of membranes made of PEBA doped with two different aminocompounds of various concentrations and their effect for CO_2 sorption and separation. Most samples indicated the CO_2 sorption improvement compared to the pristine PEBA. It strongly depends on concentration. The most significant changes were observed at MMM doped with 2.5% TEPA or 1% HDA. Samples were tested for the separation of binary CO_2/CH_4 mixture and that proved the effect on separation efficiency [2].

The basic characterization of the membrane samples was performed using a scanning electron microscope (SEM) and VegaTC software, Fourier-transform infrared spectroscopy (FTIR) and surface area and pore volume measurements. The samples were also tested for carbon dioxide capture and gas separations. Obtained results clearly showed the successful modification of PEBA2533 with selected amino-compounds, TEPA or HDA. Filling PEBA with these compounds affect surface structure, morphology and surface area.

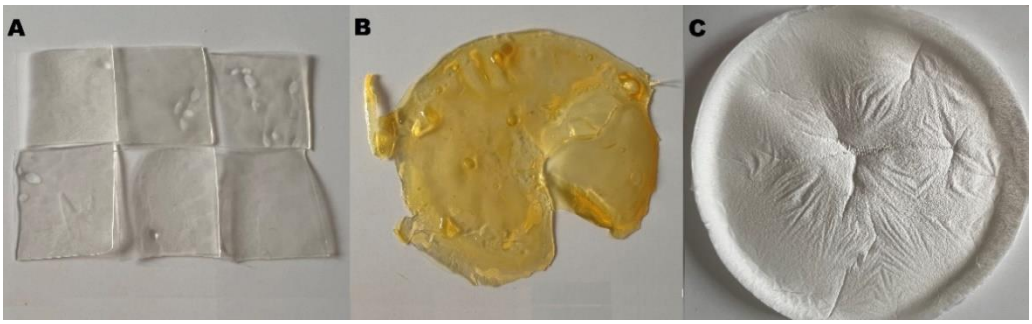

Figure 1. PEBA2533 membrane: A) pristine PEBA, B) PEBA + TEPA, 4 % and C) PEBA + HDA 2.5 %.

Research highlights:

1) Successful preparation of mixed matrix membranes containing amino-compounds.
2) The amine-doped membranes exhibited a significant increase in CO_2 sorption capacity compared with the pristine PEBA.
3) These new composites can be used for CO_2 capturing and separation.

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Polyurethane nanofiber membranes modified by amines for CO_2 capture

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[b]*Chemistry Department, Faculty of Science, J. E. Purkyne University, Czech Republic;*

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[e]*Department of Biology, Faculty of Science, Jan Evangelista Purkyne University, Czech Republic;*

[f]*Institute of Microbiology of the Czech Academy of Sciences, Czech Republic*

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The development of composite nanofibrous sorbents for CO_2 capture is primarily based on surpassing the already achieved values of sorption capacities for this important greenhouse gas. However, in this race to achieve the highest sorption values, very important issues related to real-world applicability, such as the simplicity, portability, usability and economic returns of such materials, are neglected. This research does not forget these important issues, and in this spirit, electrospinning of polyurethane (PUR Larithane) with a mixed amine TETA/TEPA modification was used to achieve them, meaning that both the electrospinning itself and the modification of the nanofibers were carried out in a single step. Not only due to computer modelling predicting the resulting interaction nature between the polymer and modifier, a 10 times more breathable PUR/TEPA 5 wt.% nanofibrous material was successfully designed and spunned simultaneously with 5 times higher CO_2 sorption capacity compared to the unmodified PUR nanofibrous membrane. Thus, this work provides a matrix and technology that is readily industrially transferable with the potential application of cyclic CO_2 capture.

Research highlights

1) Amine modified PUR membrane was prepared by one-step electrospinning technology.
2) The final expression of the sorption capacity and permeability of the PUR membrane was controlled by tuning technological parameters, solution parameters and PC modelling.
3) A 10-fold increase in breathability and a 5-fold increase in CO_2 sorption capacity were achieved.

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Isolation and Characterization of Plant Exosomes for Biomedical Applications

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Small membrane nanoparticles known as exosomes are produced spontaneously by a variety of cell types, including mammalian, fungus, and plant cells. They are able to infiltrate recipient cells and control their physiological processes because of their unique characteristics, which include the existence of plasma membrane on their surface, size (typically 30–150 nm), and the capacity to transmit different compounds, such as short RNAs or proteins. For a long time, it was unclear whether plants released exosomes; today, we know that they do [1-3]. It has been demonstrated that plant exosomes (pEXs) can penetrate the cells of other species, including human cells, where they can alter physiological functions. It has been established that pEXs have therapeutic effects on illnesses including cancer, inflammatory diseases, etc. Exosomes appear to be good drug delivery vehicles because of their optimal natural structure and features, which allow them to encapsulate the drug, cross the plasma membrane, and deliver it to the target region without triggering an immune response in the recipient organism [4–7].

A three-year student project (SGS UJEP) is funding this study. Our objective was to examine various plant materials, as well as various plants for the isolation of pEXs and to determine the best effective technique for exosome isolation. Using Dynamic Light Scattering, Nanoparticle Tracking, and biochemical protein analysis, we carried out biophysical analysis. To examine pEXs' capacity to infiltrate different cell types, Bodipy TR Ceramide was used to identify them.

Research highlights

1) We isolated tobacco-derived exosomes using two methods if isolation, namely ultracentrifugation and polyethylene glycol precipitation. Selected isolation method was used to isolate exosomes from other plant sources.
2) We determined pEXs size, concentration and protein concentration.
3) We confirmed the presence of exosomal marker.
4) We observed the uptake of labelled pEXs by mesenchymal cells and by tobacco cells.

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Biochar-Driven Phytoremediation of Complex Contaminated Sediments: Case study of *Paulwonia tomentosa*

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Numerous studies have demonstrated the viability of phytoremediation as an approach for revitalising different environmental matrices; the study focus has switched recently to the restoration of complexly (organic and inorganic origin) contaminated sites. Phytoremediation of sediments are less explored than water and soil due to heterogeneous composition and limited oxygen availability. Therefore, plant selection for sediments reclamation should be based not only on phytoremediation potential in relation to target contaminants, but also on ecological adaptability [1]. *Paulownia tomentosa* is a viable alternative plant for utilisation due to discovered tolerance to xenobitics [2] and high biomass production (50 t DM ha^{-1} yr^{-1}) even at unfavourable conditions [3].

The current study evaluated the potential of *P. tomentosa* for phytoremediation of dredged sediments complexly contaminated by HCH isomers and trace elements. Sediments were collected in Hajek, CR (GPS 50°17'31.5" N 12°53'35.2" E). The concentration of HCH isomers was 1,023 ± 56.8 µg kg^{-1}; the concentrations of Cr, Mn, Cu, Zn, Sr, and Pb exceeded MPC by up to 64.7. Dredged sediments were amended by biochar (Agmeco s.r.o., Brno, CR) in doses of 2.5, 5, and 10%. Plant height, stem diameter, dry weight (DW) of leaves, stems, and roots were measured to evaluate plant development.

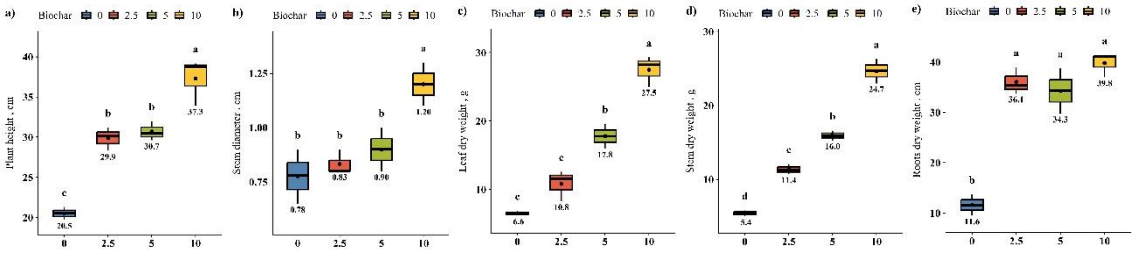

Figure 1 Physiological parameters of *P. tomentosa* grown in mixed contaminated sediments:a) plant height; b) stem diameter; c) leaf DW; d) stem DW; e) roots DW. Letters within parameter indicate a significant difference at $p<0.05$.

The application rate of 2.5% improved plant height, stem and roots DW by 45.7, 111, and 211%, respectively (Fig. 1). In 5% biochar-amended soil, leaves and stem DW were significantly higher compared to values obtained at 2.5% biochar. 10% biochar showed the highest values increasing all the parameters measured by 82.0, 54.4, 320, 357, and 243%, respectively.

Research highlights

1) *P. tomentosa* can be used to remediate complex contaminated dredged sediments.
2) Amending dredged sediments by biochar beneficial for biomass productivity.
3) Biochar application rate of 10% resulted in the greatest plant improvement.

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Molecular simulations of salts hydrates

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Classical molecular simulations have become an important tool for studying electrolyte solutions under various thermodynamic conditions. Such simulations are based on microscopic models, force fields, whose use is limited by their ability to reasonably predict solubility of the electrolyte studied and thus avoid spurious precipitation and ion clustering. Previous simulation studies have often focused on the solubility of anhydrous crystalline salts, but virtually never on crystalline hydrates, except for hydrohalite, $NaCl \cdot 2H_2O$ [1], despite there are at least 23 experimentally known different hydrates that can precipitate from alkali-halide solutions.

This work attempts to fill this gap in hydrate simulation studies by systematically investigating the ability of the best force fields selected to qualitatively capture the stability of the individual phases of various alkali-halide hydrates and to quantitatively predict their lattice parameters. First, we show that the nonpolarizable force fields studied often fail to model hydrates containing the Li^+ cations, whereas the polarizable force fields recently refined in our group [2] are able to model all the hydrates except for $LiCl \cdot H_2O$. Second, we further refine our FFs for Li^+ to yield stable $LiCl \cdot H_2O$. Third, our simulations clarify the positions of the Li^+ cations in the beta phases of $LiBr \cdot H_2O$ and $LiI \cdot H_2O$, whose distributions were previously described only as stochastic [3]. As a byproduct, a simple and reliable simulation methodology suitable also for complex polarizable models and nonorthorhombic crystal lattices is proposed and tested, based on simulations of finite crystals floating in vacuum.

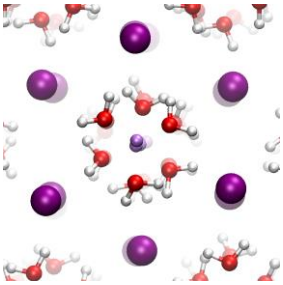

Figure 1. Snapshot from simulation of stable polarizable model of $LiI \cdot 3H_2O$.

Research highlights

1) Calculation of crystal lattice parameters for hydrates.
2) Position of Li^+ cations in beta phases of lithium bromide and iodide monohydrates.

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Impact of soil amendments on the production of *Miscanthus* × *giganteus* biomass at the slightly contaminated post-mining areas

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The robustness and physiological properties of *Miscanthus* × *giganteus* (*M*×*g*), a second-generation energy crop, allow to adapt to different soil and environmental conditions [1]. The plant has a relatively high biomass yield and cellulose content, which makes it a promising feedstock for the production of biofuels [2] and bioproducts: fibres, insulation materials, and paper [3]. Cultivation of *M*×*g* on slightly contaminated or marginal soils offers environmental and economic advantages.

The aim of this research was to utilize *M*×*g* in the post-mining soil treated by various amendments, to monitor the bio bioparameters, and to study the change in the soil nematode communities during vgetation. wo *M*×*g* fields were established in 2020 and 2021 on the former post-mining land in Chomutov, the Czech Republic. The field of 2020 (F2020) was supplemented with NPK, biochar + NPK (BNPK), digestate (D), and sewage sludge (SS). The field of 2021 (F2021) was supplemented with biochar in two dosages of 5 and 10% (BD1 and BD2), D, SS, and hemicellulosic waste (HW). The bio parameters of *M*×*g* were assessed during three growing seasons for F2020 and two growing seasons for F2021. The following parameters were monitored: the number of plants per plot, plant height, and biomass dry weight at harvest (DW).

Results showed that for F2020, the number of *M*×*g* plants in soil supplemented with D was highest for the first and third vegetation. In 2021 and 2022 the highest biomass DW was detected when *M*×*g* grew in the control soil. However, in 2023 the tendention changed and highest biomass DW was detected for *M*×*g* growing in D amended soil. For F2021, the highest number of plants was recorded in the plot supplemented with BD2. In 2022, the DW of biomass was significantly higher when plant grew in D amended soil compared with DW biomass of plants amended by other amendments, the exception fixed only for BD1. There was no significance difference in biomass DW values for "green" harvest in 2022 and "brown" harvest in 2023 in between different soil treatments. During the first 2021 vegetation the nematode communities were assessed for F2021. Results showed [4] that SS and D favoured a more stable maturity status of the nematode community, and the effects of soil amendment by BD1, BD2, and HW on nematodes communities were controversial.

Research highlights

1) D increased biomass yield for F2020
2) BDs increased biomass yield for F2021
3) The nematode community associated with *M*×*g* was sensitive to the type of amendments applied

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Straight Channel Microfluidics for Viscoelastic Exosome Separation – Influence of Geometry and Materials

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Exosomes, membrane vesicles ranging from 30 to 200 nm in size and secreted by nearly all mammalian cells, have gathered significant attention in recent years due to their substantive informational cargo, including proteins, microRNAs, and DNAs, as well as their potential role as biomarkers. Alternative methods of exosome isolation that could substitute ultracentrifugation, which has numerous limitations, are also widely discussed. Inertial microfluidics employing viscoelastic separation in non-Newtonian fluids with sheath flows have emerged as promising candidates. However, as factors such as channel geometry, fluid viscosity, and flow rate significantly influence the final separation, the design and application of these straight microfluidic channels are not as straightforward as we would hope.

To address these challenges, we developed an accurate numerical model representing the principal forces acting on exosomes in straight microfluidic channels. We conducted experiments using fabricated chips with varying channel dimensions and identified an optimal approach for designing and employing these channels for exosome separation in several key applications. Additionally, as polydimethylsiloxane (PDMS) may present problems due to its deformability at higher pressures, leading to alterations in channel geometry, we simultaneously fabricated chips from a rigid, ultraviolet and heat-cured thermoset polymer, Ostemer, and compared the resulting separation efficiencies. We propose that viscoelastic microfluidics may serve as a compelling alternative to conventional exosome separation techniques.

Research highlights

1) Microfluidic alternatives to conventional exosome isolation were explored.
2) A numerical model for nano/microparticle forces in channels was developed.
3) Optimal approaches for exosome separation were identified through experiments.
4) Separation efficiencies of PDMS and Ostemer chips were compared.

Determination of *Mercurialis ovata* and *Mercurialis perennis* hybrids according to morphological features and genome size

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It is thought that interspecific hybridization and polyploidization are significant sources of variability. Within the genus *Mercurialis*, hybridization and polyploidization is well known, but primarily in annual species. In this study, new potential hybrids of the North Bohemian rhizomatous monoecious perennials *M. annua* and *M. perennis* have been proposed. Despite their similarities, these two species have distinct morphological and ecological differences that make them easily distinguishable. However, recent studies have suggested that hybridization between these two species may be possible, leading to the creation of new hybrids with unique traits and potential benefits, mainly in the field of phytoremediation. One of the parental species, *Mercurialis perennis* has exhibited a remarkable ability to tolerate and accumulate heavy metals, such as mercury, cadmium, lead, and zinc, in their tissues [1].

In the Ore Mountains (Krušné hory), non-standard phenotypes of perennial Mercurialis were observed, suggesting possible interspecific hybridization or even polyploidization of the original species. These hybrids were identified at the beginning of the 20th century as *Mercurialis x paxii* Grebn and *M. longistipes* (Borbás) Holub, but a detailed description is missing [2].

For the purpose of this study, standard parental plants (*M. ovata* as well as *M. perennis*) with distinct phenotypes were collected at the locality of Skalka u Trebutiček, district of Litoměřice. These plants show stable morphological characteristics and served as standards for the establishment of the genome size of the hybrids.

Samples of *M. perennis* possess 6,70 ± 0,22 pg/2C. In *M. ovata*, 2,98 ± 0,12 pg/2C. Plants that differed in the morphology of their leaves were identified as plausible hybrids with a mean genome size of 4,89 ± 0,04 pg/2C, but measurements of leaf morphological characteristics suggest that the situation might be much more complex.

Nevertheless, the hybrid could show even better phytoremediation potential than the parental species. For this reason, it is necessary to distinguish and describe parental species and hybrids in detail, using genome size and morphological characteristics.

Research highlights

1) Ore Mountains are possible area for unique *Mercurialis* hybridization .
2) New *Mercurialis* hybrids may enhance phytoremediation potential
3) Distinct genome size in hybrids indicates complex origin.

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