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Faculty of Environment

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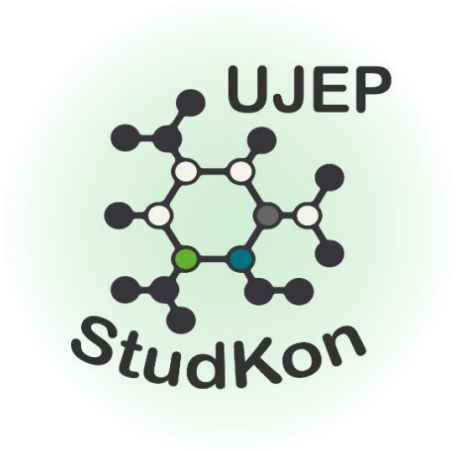


# BOOK OF ABSTRACTS

## 7th Conference of Natural Sciences and Technical PhD study programmes at UJEP

## StudKon 2024

24. – 25. 6. 2024

Centre of Natural and Technical Sciences

J. E. Purkyně University in Ústí nad Labem

http://www.studkon.ujep.cz

# StudKon 2024 programme:

| **MONDAY 24. 6. 2024** | |
|---|---|
| **Registration** | **8:00 - 9:00** |
| **Morning sessions** | **9:00 – 14:00** |
| 9:00 – 9:15 | Opening and welcome session |
| 9:15 – 10:35 | **Talks session 1**<br>9:15 Oksana Batkivska<br>9:35 Ladislav Bříza<br>9:55 Lenka Vavrincová<br>10:15 Anna Kokavcová |
| 10:35 – 11:10 | Coffee break |
| 11:10 – 12:30 | **Talks session 2**<br>11:10 Jan Čundrle<br>11:30 Abdulmannan Rouhani<br>11:50 Kristýna Šedivá<br>12:10 Václav Harrandt |
| 12:30 – 14:00 | Lunch break |
| **Afternoon sessions** | **14:00 – 18:00** |
| 14:00 – 15:20 | **Talks session 3**<br>14:00 Jakub Neumann<br>14:20 Jiří Brejcha<br>14:40 Miroslava Sincak<br>15:00 Michaela Kocholatá |
| 15:20 – 15:40 | Taking photo together |
| 16:00 – 18:00 | **Poster session** + light refreshment |
| **Evening programme** | **18:00 – 22:00** |
| 18:00 – 19:00 | Invited talk: doc. Mgr. Martin Veselý, Ph.D.: Historical development of brewing and drinking beer in the region. (talk will be in Czech, slides in English). |
| 19:00 – 22:00 | Barbecue |

| **TUESDAY 25. 6. 2024** | |
|---|---|
| **Morning sessions** | **9:30 – 14:00** |
| 9:30 – 10:50 | **Talks session 4**<br>9:30 Pavlína Mimrová<br>9:50 Robert Ato Newton<br>10:10 Kateřina Hamalová<br>10:30 Anna Paříková |
| 10:50 – 11:20 | Coffee break |
| 11:20 – 12:40 | **Talks session 5**<br>11:20 Saddam Hussain Mubin<br>11:40 Eva Štěpanovská<br>12:00 Tereza Dušková<br>12:20 Jan Štěpka |
| 12:40 – 13:40 | Lunch break and technical break |
| 13:40 – 14:00 | The Miroslav Broul award ceremony and conclusion of the conference |

# List of participating PhD students and their contributions:

**Talk session 1**

- **Oksana Batkivska** *(1st year, Applied nanotechnology, PřF UJEP):* Exosomal Galectins: Key Players in Cell Proliferation and Tumor Progression
- **Ladislav Bříza** *(1st year, Environmental chemistry and technology, FŽP UJEP):* Novel approach to recovery of $Li_2CO_3$ from spent lithium batteries
- **Lenka Vavrincová** *(1st year, Applied analytical and bioanalytical chemistry, UCM Trnava, Slovakia)*: Carbonized sewage sludge as a renewable source of phosphorus for plants
- **Anna Kokavcová** *(1st year, Computer modelling in science and technology, PřF UJEP)*: Modeling of Heat Transfer in Granular Media: Influence of mixing dynamics and material properties

**Talk session 2**

- **Jan Čundrle** *(1st year, Environmental chemistry and technology, FŽP UJEP)*: Study of hydrolysis of sulfonylurea herbicides on nanoceria
- **Abdulmannan Rouhani** *(1st year, Landscape reclamation and ecosystem services, FŽP UJEP):* Human health risk assessment of potentially toxic elements in urban green spaces (Case study: Ústí nad Labem-centrum)
- **Kristýna Šedivá** *(1st year, Landscape reclamation and ecosystem services, FŽP UJEP):* Enhancing Seed Germination and Photosynthetic Efficiency in Poppy (Papaver somniferum L.) Using Cold Plasma Treatment
- **Václav Harrandt** *(2nd year, Computer modelling in science and technology, PřF UJEP):* Multiphase Flow Simulations: Exploring Bubble Dynamics with Volume of Fluid Method

**Talk session 3**

- **Jakub Neumann** *(2nd year, Applied ion technology, PřF UJEP):* Characterization of individual microscopic particles using a combination of micromanipulation, microscopy and microanalytical methods
- **Jiří Brejcha** *(3rd year, Engineering technology, FSI UJEP):* Evaluation of the influence of the elastomeric matrix on the properties of a rubber compound containing sustainable raw materials
- **Miroslava Sincak** *(3rd year, Biotechnology, UCM Trnava, Slovakia):* Impact of low-frequency electromagnetic field on yeast Saccharomyces cerevisiae growth
- **Michaela Kocholatá** *(3rd year, Applied nanotechnology, PřF UJEP):* Isolation and Characterization of Plant Exosomes for Biomedical Applications

**Talk session 4**

- **Pavlína Mimrová** *(3rd year, Computer modelling in science and technology, PřF UJEP):* Molecular modeling of alkali halides using phase-transferable models: aqueous solutions, anhydrous crystals, crystalline hydrates, molten salts
- **Robert Ato Newton** *(4th year, Environmental chemistry and technology, FŽP UJEP):* Biochar Assisted Phytoremediation with Miscanthus × giganteus in Trace Elements Contaminated Soil
- **Kateřina Hamalová** *(3rd year, Applied nanotechnology, PřF UJEP):* Chitosan/alginate biofilms with deep eutectic solvents in Microbial Fuel Cells
- **Anna Paříková** *(3rd year, Applied nanotechnology, PřF UJEP):* Computational Fluid Dynamics Studies for Optimizing Stem Cells Cultivation

**Talk session 5**

- **Saddam Hussain Mubin** *(master student, Hydroscience and engineering, TU Dresden, Germany):* Assessment of Biochars Properties Prepared from Different Feedstocks and Their Prospects as Carbon-capturing and Sequestering Construction Materials
- **Eva Štěpanovská** *(3rd year, Applied ion technology, PřF UJEP):* Modification of graphene-like materials and polymer thin films with energetic ions for their application in energy storage
- **Tereza Dušková** *(4th year, Applied nanotechnology, PřF UJEP):* Harnessing Perfluorocarbon-Based Nanocarriers for Rhodium (III) NHC Complex Delivery: Synthesis, Characterization, and Cytotoxicity Evaluation
- **Jan Štěpka** *(4th year, Applied nanotechnology, PřF UJEP):* Influence of $CeO_2$ nanoparticles and alginite particles on microbial communities in hemp rhizosphere and soil: DNA sequencing and bioinformatics approach

**Poster session**

- **Slavomír Adamec** *(3rd year, Environmental chemistry and technology, FŽP UJEP)*: Distinguishing of anthropogenic contamination and natural geogenic anomaly in soils in Northwestern Bohemia
- **Adeyemi Adejare** *(master student, Hydroscience and engineering, TU Dresden, Germany):* The Effect of Ryegrass on Enhancing Soil Carbon and Nutrients Storage
- **Gabriela Bílková** *(3rd year, Environmental chemistry and technology, FŽP UJEP):* Birch foliar analysis for mapping weak soil contamination by zinc
- **Katrien Boonen** *(3rd year, Environmental chemistry and technology, FŽP UJEP):* The effect of acidifying pollution on spruce growth
- **Šárka Dědičová** *(3rd year, Computer modelling in science and technology, PřF UJEP):* External electric field induced structural change of oligo(ethylene glycol) in explicit solvents: A molecular dynamics study

- **Jaffar Iqbal** *(1st year, Landscape reclamation and ecosystem services, FŽP UJEP):* Effect of variety on the chemical composition of the grain of spelt (Triticum. spelta L.) wheat
- **Jaroslava Jarolímková** *(2nd year, Applied nanotechnology, PřF UJEP):* Liquid exfoliantion of molybdenum disulfide for hydrogen evolution reaction
- **Alexandra Kinder** *(1st year, Molecular biology, UCM Trnava, Slovakia):* Variability of durum wheat (Triticum durum) in intake and accumulation of zinc
- **Petr Panuška** (5th year, *Applied nanotechnology, PřF UJEP):* A perfusion system for testing of the effects of electrical field on osteogenic differentiation of human mesenchymal stem cells
- **Muhammad Roman** *(1st year, Landscape reclamation and ecosystem services, FŽP UJEP):* Temporal Trends in Winter Wheat Yields: The Role of Fertilization, Proceeding Crop and Weather Over Decades of Field Experiments
- **Michal Syrový** (3rd year, *Applied nanotechnology, PřF UJEP):* Dual-Functional Nanofibrous Materials for Enhanced $CO_2$ Capture and Photocatalytic Conversion
- **Martin Šulc** (*4th year, Environmental chemistry and technology, FŽP UJEP):* Gypsum technology of separation $Li_2CO_3$ from Zinnwaldite mineral
- **Vojtěch Trnka** *(1st year, Applied nanotechnology, PřF UJEP):* Microfluidic Blood-Brain-Barrier model for extracellular vesicles transport studies
- **Muhammad Zubair** *(1st year, Landscape reclamation and ecosystem services, FŽP UJEP):* Miscanthus x giganteus: An Industrial Crop for Phytoremediation of Pharmaceuticals from Hospital Wastewater in Soil

# Talks session 1
# (MO 9:15 – 10:35)

# Exosomal Galectins: Key Players in Cell Proliferation and Tumor Progression

Oksana Batkivska[a,*], Michaela Kocholatá[a], Helena Medunová[a], Jan Malý[a], Olga Šebestová Janoušková[a]

[a]*Centre of Nanomaterials and Biotechnology, J. E. Purkyně University in Ústí nad Labem, Czech Republic*
**Presenting author, e-mail: batkivskao@g.ujep.cz 1st year of PhD, Applied Nanothechnology*

Exosomes are nanovesicles produced by all body cells, including tumor's. Exosomes have characteristic features as regulated formation, specific makeup of cargo, cell-target specificity and exosomes play major roles in cell-cell communication, migration, proliferation, angiogenesis, immune response and pathological metastatic growth. Moreover, along with the study of exosomes in context of cancer, it is important to study factors, which can influence tumor progression, development of neovasculation and immunomodulation. One of them are galectins, which are highly expressed by tumor cells and have high potential as non-invasive diagnostic, prognostic and effector markers of cancer.

We hypothesize that the isolation, measuring and investigation of galectin-containing exosomes from patients with glioblastoma, an aggressive primary brain tumor characterized by increasingly resistant neoplasm re-growth, may provide new insights into pathogenesis and novel approaches for diagnosis and therapy via exosomes.

Research highlights

1) Isolated blood's exosomes from healthy volunteers, patients before and two times during therapy, as well as exosomes from patient tumor tissue.
2) Characterized the size, concentration and protein content of exosomes using Nanoparticle Size Analyzer and Dynamic light scattering etc.
3) Evaluated the difference in expression level of galectins between control group and groups of patients by Western blotting.
4) Investigation of migration and proliferation of primary tumor cells under the influence of exogenous exosomes is our next crucial tasks.

References

[1] Wang, X., Tian, L., Lu, J., & Ng, I. O. (2022). Exosomes and cancer - Diagnostic and prognostic biomarkers and therapeutic vehicle. Oncogenesis, 11(1), 54. https://doi.org/10.1038/s41389-022-00431-5

[2] Bänfer, S., & Jacob, R. (2020). Galectins in Intra- and Extracellular Vesicles. Biomolecules, 10(9), 1232. https://doi.org/10.3390/biom10091232

[3] Touat, M., Idbaih, A., Sanson, M., & Ligon, K. L. (2017). Glioblastoma targeted therapy: updated approaches from recent biological insights. Annals of oncology : official journal of the European Society for Medical Oncology, 28(7), 1457–1472. https://doi.org/10.1093/annonc/mdx106

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# Carbonized sewage sludge as a renewable source of phosphorus for plants

Lenka Vavrincová[a,*], Martin Pipíška[b], Jana Urbanová[b], Miroslav Horník[a]

[a]*Institute of Chemistry and Environmental Sciences, University of SS. Cyril and Methodius in Trnava, Slovakia*

[b]*Faculty of Education, Trnava University in Trnava, Slovakia*

**Presenting author, e-mail: vavrincova4@ucm.sk 1st year of PhD, Applied Analytical and Bioanalytical Chemistry*

As phosphorus is a crucial macroelement for supporting plant growth, increasing demands for food and bioenergy lead to the use of rock phosphate for the production of conventional phosphorus (P) fertilizers. Overproduction of P fertilizers is associated with two environmental problems: water eutrophication and possible depletion of non-renewable P resources [1]. It is therefore important to look for other sources of phosphorus, whereby recycling of phosphorus from e.g. sewage sludge appears to be a suitable alternative [2].

In our research, we used carbonized sewage sludge (SS biochar) as a source of P for green roof vegetation and investigated total phosphorus (TP) leaching from experimental green roof plots over a period of three years. Commercial substrate without SS biochar was used as a control treatment, and the same substrate was amended with 10 % and 20 % of SS biochar (SB10 and SB20), each treatment in four replicates. TP concentrations in runoff from green roof plots ranged between 0.04 – 1.63, 0.18 – 2.00, and 0.03 – 1.71 mg/L for SB0, SB10, and SB20, respectively. From Fig. 1, it is evident that TP concentrations were highest after the initial leaching (> 1.5 mg/L) compared to the subsequent progression. However, we also observed TP content in the runoff at the end of the study, indicating that there was no rapid leaching of TP and SS biochar represents a long-term and renewable source of phosphorus for plants, and does not pose a risk for water eutrophication.

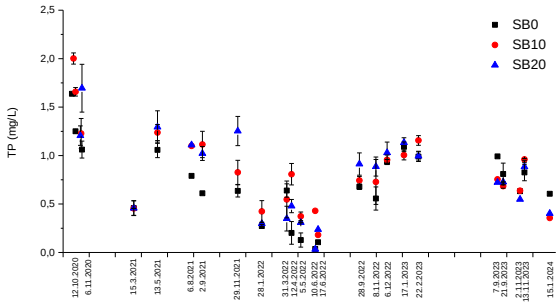


**Figure 1** Average (±SE) total phosphorus (TP) concentrations in runoff from experimental green roof plots containing substrate without biochar (SB0), and substrates with SS biochar (SB10 and SB20).

Research highlights

1) Experimental green roof plots showed the first-flush behavior for P leaching.
2) TP concentrations in runoff from SB10 and SB20 were slightly higher than from SB0.
3) Carbonised SS serves as a long-term source of P for plants.

Acknowledgement: Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V02-00018.

References

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[2] LIN, H., WANG, Y. and DONG, Y. A review of methods, influencing factors and mechanisms for phosphorus recovery from sewage and sludge from municipal wastewater. J. Environ. Chem. Eng., 2024, 12, 111:657.

# Modeling of Heat Transfer in Granular Media: Influence of mixing dynamics and material properties

Anna Kokavcová[a,b*], Martin Svoboda[a], Jaromír Havlica[a,b]

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

[b]*Institute of Chemical Process Fundamentals, The Czech Academy of Sciences, Czech Republic*

**Presenting author, e-mail: annkokavcova@gmail.com, 1st year of PhD, Computer Modelling in Science and Technology*

Heat transfer plays a crucial role in various industrial applications, including power generation, chemical processing, and manufacturing. Understanding the mechanisms of heat transfer and maximizing its efficiency is essential for optimizing industrial operations and reducing energy consumption. Recent advancements in both experimental studies and computational models have significantly enhanced our understanding of this phenomenon. Among these, the Discrete Element Method (DEM) has emerged as a leading computational technique, offering a viable alternative to direct physical measurements [1]. DEM simulations model the granular flows by calculating force and heat energy balances for each individual particle. In scenarios where gas phase conduction and convection are minimal, and radiation is negligible due to low temperatures, solid phase conduction becomes the dominant mode of heat transfer. This type of heat transfer is affected by factors such as contact area and contact time, which depend on material properties like Young's modulus and the rotational speed of the mixing device [2].

This study uses DEM simulations to investigate the heat transfer dynamics within a vertically oriented cylindrical mixer equipped with two flat blades positioned at a 45-degree angle and paired with heating jackets. The research examines how varying the mixer's rotational speed affects heat transfer, with a detailed analysis of particle motion to determine the influence of primary and secondary flow patterns on thermal efficiency. In addition, the study examines how changes in Young's modulus affect heat transfer at different dynamical conditions. Detailed descriptions of the simulation parameters and their effects on heat transfer efficiency are provided to enhance the reproducibility and applicability of the results. Initial results indicate that both agitation speed and particle mechanical properties significantly affect heat transfer efficiency, suggesting potential optimization strategies for industrial mixing processes.

Research highlights

1) Heat transfer in granular media is studied using DEM simulations.
2) The influence of mixing dynamics and material properties is analyzed.
3) The influence of primary and secondary flow on heat transfer is investigated.

References

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Acknowledgements

This work was supported by the Internal Grant Agency of Jan Evangelista Purkyně University in Ústí nad Labem (projects no. UJEP-SGS-2023-53-005-3 and UJEP-IGA-2024-53-003-2).

# Talks session 2
# (MO 11:10 – 12:30)

# Study of hydrolysis of sulfonylurea herbicides on nanoceria

Jan Čundrle[a,b,*], Martin Šťastný[b] and Jiří Henych[a,b]

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[b]*Institute of Inorganic Chemistry of the Czech Academy of Sciences, Husinec-Řež, Czech Republic*

**Presenting author, e-mail: cundrle@iic.cas.cz, 1st year of PhD, Environmental Chemistry and Technology*

Due to its unique properties, nanoceria ($CeO_2$) is a promising material for the catalytic hydrolysis of a wide range of organic compounds such as organophosphates [1], sulfonamides [2] and other various ester compounds that have not been studied in more detail so far. One of the large group of industrially utilized esters - sulfonylurea compounds, are widely used as herbicides for weed control or drugs against type II Diabetes Mellitus [3]. In this work, we have focused on the hydrolytic decomposition of three different sulfonylurea herbicides (nicosulfuron, amidosulfuron, and metsulfuron-methyl) in aqueous solution using three different nanoceria samples prepared by simple precipitation methods. The nanomaterials differ significantly in their physicochemical properties and reactivity. It was found experimentally, that only one nanoceria sample shows the unique degradation activity towards investigated herbicides. At least two different degradation products were identified by HPLC/DAD method using reference standards (see figure 1). Further investigation will be performed with aid of LC-MS and also computational chemistry methods (e.g., DFT) in order to describe and comprehend the unique reactivity and catalytic activity of $CeO_2$-based nanomaterials.

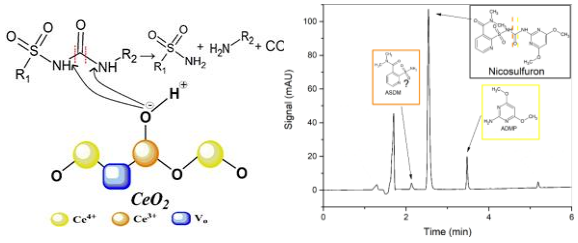


**Figure 1**: (left) General scheme for hydrolysis of sulfonylurea herbicides on $CeO_2$ surface and (right) the representative HPLC chromatogram showing nicosulfuron degradation products formed after the reaction with $CeO_2$ nanoparticles.

Research highlights

- Hydrolytic decomposition of sulfonylurea herbicides on $CeO_2$ was observed for the first time.
- Several degradation products were identified with HPLC/DAD.
- Degradation ability is strongly dependent on the surface properties of $CeO_2$.

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# Human health risk assessment of potentially toxic elements in urban green spaces (Case study: Ústí nad Labem-centrum)

Abdulmannan Rouhani [a,*], Robert Ato Newton [a], Karim Suhail Al Souki[a], Valentina Pidlisnyuk[a], Michal Hejcman[a]

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

**Presenting author, e-mail: a.rohani70@gmail.com 1st year of PhD, study program: Landscape reclamation and ecosystem services*

Green spaces are well documented for socio-economic and environmental benefits in urban areas by enhancing the natural environment and human health. Despite this, urban areas become the sources of various soil pollutant elements accumulated in the soil. Soil pollution by potentially toxic elements (PTE) is a global environmental issue that potentially harms the ecosystem and human health. In this study, 60 samples were collected from the topsoil of different urban green spaces (UJEP Campus, UJEP Koleje, Mánesovy sady, Vrchlického sady, and Městské sady) in Ústí nad Labem-centrum. Herein, concentrations of As, Cu, Pb and Zn in surface soil were measured to evaluate their potential health risks to adults and children. Human health risk assessment model was utilized to calculate the potential health risks (including non-carcinogenic and carcinogenic risks) via different pathways including ingestion, inhalation and dermal contact based on U.S. Environmental Protection Agency (US EPA) guild lines [1, 2]. Results indicated that highest concentration of Cu (77.08 mg/kg), Zn (192.58 mg/kg), Pb (63.25 mg/kg) were detected in Mánesovy sady, while highest level of As (28.33 mg/kg) was recorded in Městské sady. Hazard index showed no health risk for adults caused by studied PTE concentrations in the green space soils of Ústí nad Labem-centrum. However, potential adverse non-cancer health effects of As for children were observed in Městské sady and Mánesovy sady. No health risks were recorded for Cu, Pb and Zn in the study area for both adults and children.The carcinogenic risk values of Cu for children were higher than the safe value ($1 \times 10^{-6}$) in Městské sady and Mánesovy sady, indicating that receptors in these parks might have a significant potential health risk. While carcinogenic risk values of Cu for adults were within acceptable potential health risk from Městské sady and Mánesovy sady. Other studied elements did not show any carcinogenic risks in the study area.Children had larger health risks in non-carcinogenic and carcinogenic risks than adults who may be associated with their behavioral and physiological features.

Research highlights

1) Mánesovy sady was the most polluted spot in the study area in terms of Cu, Zn, and Pb.
2) As had potential adverse non-cancer health effects for children in Městské sady and Mánesovy sady.
3) Cu showed higher carcinogenic risk values for children in Městské sady and Mánesovy sady.
4) Children had larger health risks in non-carcinogenic and carcinogenic risks than adults.

References

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# Enhancing Seed Germination and Photosynthetic Efficiency in Poppy (*Papaver somniferum* L.) Using Cold Plasma Treatment

Kristýna Šedivá [a,b*], Hana Auer Malinská [b], Jakub Perner [b], Jindřich Matoušek [b]

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

[b]*Faculty of Science, Jan Evangelista Purkyně University in Ústí nad Labem, Czech Republic*

**Presenting author, e-mail: sedivakristyna@email.cz, 1st year of PhD, study program: Landscape reclamation and ecosystem services*

Seed germination is a critical issue in horticulture and agriculture. Seed germination and biomass production is essential in the context of a growing global population and changing environmental conditions. Cold plasma treatment offers a promising, environmentally friendly method for enhancing seed germination and plant growth. This study investigated the impact of cold plasma treatment on seed germination, leaf pigment content, and the primary phase of photosynthesis in poppy (*Papaver somniferum* L.). The results demonstrated that cold plasma treatment significantly enhanced seed germination across all tested variants. The highest germination rate was achieved with the 150W treatment, showing a 36 % increase compared to the control. Additionally, there was an increase in germination energy and improvement in chlorophyll fluorescence parameters, particularly in the 40W and 100W variants, where the maximum quantum yield of PSII (FV/FM) was 1,62 % higher than the control. These findings suggest that cold plasma treatment is an effective method for improving germination and physiological parameters of poppy seeds, which could have significant agricultural applications.

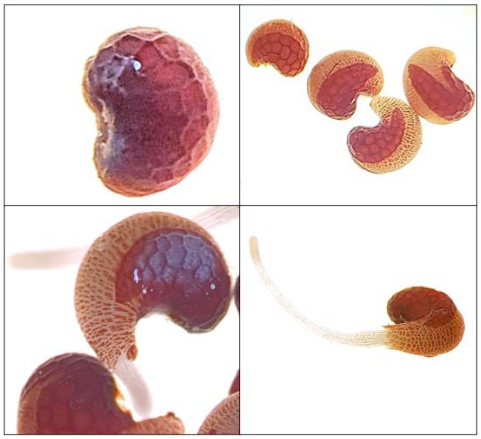

**Figure 1** Germination of poppy seeds treated with cold plasma

Research highlights

1) Cold plasma treatment enhances germination of common poppy seeds by up to 36%.
2) Enhanced germination energy observed with cold plasma treatment.
3) Chlorophyll fluorescence parameters improved by cold plasma.
4) Cold plasma positively affects leaf pigment content.
5) Environmentally friendly alternative to chemical seed treatments.

# Multiphase Flow Simulations: Exploring Bubble Dynamics with Volume of Fluid Method

Václav Harrandt[a,b*], Tereza Semlerová[b], Mária Zedníková[b], Jaroslav Tihon[b], Jaromír Havlica[a,b]

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

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**Presenting author, e-mail: vaclavharrandt@seznam.cz 2nd year of PhD, Computer Modelling in Science and Technology*

Four basic configurations of gas and liquid phases, namely bubbly, slug, annular, and churn flow regimes, can be encountered in gas-liquid flow in channels [1]. It is of interest to the scientific community to investigate these flows, as knowledge of their fundamental behavior is needed in many industrial or energetic sectors. This knowledge can help design appropriate operating conditions for devices such as heat exchangers, nuclear reactors, or membrane separation modules.

This study delves into the dynamics of Taylor bubbles and the collision of a bubble with a vortex ring. The former case represents the three-phase interaction between the channel wall, liquid and gas, and its understanding can be essential to prevent the membrane fouling or the flow-induced corrosion. The insights from the latter case, which serves as a model liquid-gas interaction, can be the predictive criterion for whether the initial mother bubble will break up into the daughter bubbles or not [2], and this process can therefore be used as an idealized model of turbulent bubbly flow.

The current endeavor aims to establish a robust simulation cornerstone that, together with experimental investigations, explores the aforementioned issues. The simulations were performed with the OpenFOAM software using the finite volume method for discretization and the Volume of Fluid (VOF) method for the multiphase flow scenarios. In the case of Taylor bubble flow, rectangular channels with higher aspect ratio values have been studied. An efficient procedure has been implemented that allows the simulation of Taylor bubbles in a moving reference frame. The experiments were performed using a Plexiglas channel with modifiable geometry, and bubble motion was recorded using a high-speed camera. The primary parameters studied included bubble velocity and liquid film thickness for different channel inclinations and geometries. In the case of bubbles interacting with the vortex ring, the interaction process was recorded by high-speed cameras during the experimets and complemented by the PIV method to evaluate the velocity field in the plane. Regarding the simulations, the main advantage is that the results can be evaluated in 3D space and also with a better resolution. Attention has been paid to quantities characterizing the geometric parameters and dynamics of both objects. The interaction also led to the determination of the number of daughter bubbles formed by the collapse of the mother bubble.

Research highlights

1) An efficient procedure for simulating Taylor bubbles is implemented.
2) Taylor bubble flow in rectangular channels with higher aspect ratios is studied.
3) Geometric and dynamic parameters of the vortex ring are evaluated.
4) The collision of the vortex ring with the bubble is modeled.

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# Talks session 3
# (MO 14:00 – 15:20)

# Characterization of individual microscopic particles using a combination of micromanipulation, microscopy and microanalytical methods

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Characterization of individual particles plays a vital role in nuclear forensic analyses. These analyses are performed mainly for the purposes of nuclear safeguards in accordance with the Treaty on the Non-Proliferation of Nuclear Weapons (NPT) [1]. The particles are gathered as dust by swiping surfaces at places of interest during inspections, environmental monitoring or criminal investigations. They are then extracted from the swipes onto a planchet or another type of planar substrate, depending on the extraction method. During their extraction many of the particles get clustered together, but some of them remain sufficiently separated to allow for their individual extraction for more detailed analyses. Individual particles are of the utmost interest, because each particle contains unique information about its origin and history. Their sizes range from tens of microns down to a single micron or less. Due to their size, a sufficiently selective and precise method of manipulation is required to access that information reliably.

This work focuses on the development of single-particle micromanipulation methods for the purposes of nuclear forensic analyses. Two approaches are demonstrated using test particles prepared from natural uranium (NU) powder. The first approach – electrostatic micromanipulation, based on previous works utilizing electrostatic forces between a manipulator needle and a particle on a flat substrate [2, 3], has been adapted for an upright optical microscope. It is simple, relatively fast, but its reliability and precision depend strongly on the needle tip definition. Despite that limitation, transfer of NU particles with precision better that 10 μm has been achieved even without a well-defined needle tip. The second approach – FIB micromanipulation, utilizes electron microscope quipped with focused ion beam (FIB), gas injection system (GIS) and a nanomanipulator, to attach and detach NU particles to and from the manipulator needle with submicron precision, mainly at the cost of speed. The transfers have been verified by a combination of optical microscopy, SEM and EDS.

Research highlights

1) Electrostatic transfer of 2-10 μm NU particles onto C-nanorods grown using FIB.
2) Electrostatic aggregation of 2-10 μm NU particles on a flat surface spaced less than 10 μm apart.
3) Transfer of 1-2 μm NU particles in an electron microscope using FIB.

Acknowledgements: Experimental work was done using the analytical infrastructure of Research Centre Řež, supported by CVŘ: Open Access CICRR (project no. PP0994)

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# Evaluation of the influence of the elastomeric matrix on the properties of a rubber compound containing sustainable raw materials

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Rubber is a material that offers multiple applications, such as cushioning or insulation. The most significant percentage is used for tyre manufacturing. Every year, the number of tyres discarded at the end of their useful lifecycle increases. If not managed correctly, causes environmental issues at various levels due to extensive natural degradation. The vulcanisation process that rubber undergoes in its manufacture causes a structure with a high degree of cross-linking, making its recycling difficult.

Circular economy is one of the most essential European Community policies. The sustainability of rubber formulations has become a priority of research and development activities in polymer science and industry.

Utilizing different recycled materials in virgin compounds is a direct way to achieve this target. Other sustainable and recycled materials were used in the variable elastomer matrix of agriculture tyre tread compound. The study also aimed to characterize the impact of combining the elastomer matrix and type of additive material.

Research highlights

1) Impact characterization of the elastomer matrix combination and additive material type.
2) Identifying potential ways of utilization recycled cured rubber materials
3) Potential elimination of rubber waste.
4) Characterization of parameters within the ageing period.

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# Impact of low-frequency electromagnetic field on yeast *Saccharomyces cerevisiae* growth

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Nowadays, organisms face challenges from anthropogenic electromagnetic fields, the overall impact of which remains poorly understood. While research on electromagnetism primarily focuses on human health risks, the adaptation of microorganisms to electromagnetic stress is relatively unexplored [1].

In our study, we investigated the effects of a wide range of magnetic fields (0.15-2.4 mT) on the growth on *Saccharomyces cerevisiae* under various exposure times induced by static and alternating electric fields. We found that weaker electromagnetic fields have negligible effects on yeast growth but impact the progression of the cell cycle by 17 hours. Conversely, stronger electromagnetic fields stimulated yeast growth by 5-30%, depending on the exposure time and field parameters. The results showed that 10 and 15 mT magnetic fields not only significantly boosted and sped up biomass production (by 38-70%), but also accelerated overall metabolism, accelerating glucose, oxygen, and nitrogen consumption, by 1-2 hours.

Additionally, we observed that exposure to hypomagnetic fields (weaker than the Earth's magnetic field) inhibited yeast growth, resulting in growth reductions ranging from 10% to 30%. These findings suggest the potential negative consequences of the absence of a magnetic field on organisms during interplanetary flights [2].

Despite preliminary research on electromagnetic fields, the impact of electromagnetism on microorganisms remains poorly explored and may represent a significant stressor that can be utilized to control their growth. The work was supported by financial by projects VEGA 1/0018/22 and FPPV-32-2023.

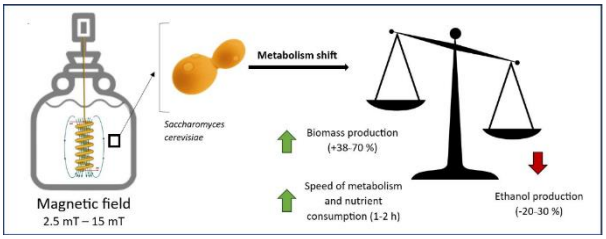


**Figure 1** The effect of electromagnetic field on biomass and ethanol production of *S. cerevisiae*

Research highlights.

1) Magnetic fields enhanced the biomass production rather than alcohol production.
2) Fields of 10 and 15 mT offer novel approach to biotechnological process control.
3) Hypomagnetic field inhibits the microbial growth.

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# Isolation and Characterization of Plant Exosomes for Biomedical Applications

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Recent interest in plant exosomes (pEXs) from edible sources has surged due to their efficient delivery of bioactive molecules into mammalian cells. Characterized by their specific properties, including size and plasma membrane surface, these vesicles possess unique capabilities for biomolecule transfer, facilitating entry into recipient cells and modulation of cellular processes. Additionally, they can be enriched with secondary metabolites that exhibit immunomodulatory, antibacterial, or anti-inflammatory effects.

Our research investigates the properties and potential of *Nicotiana tabacum*-derived pEXs as drug delivery vehicles. We conducted a comparative analysis of pEXs yields from apoplastic fluid, sterile calli, and suspension cultures to identify the optimal plant material for vesicle isolation. Subsequent experiments focused on assessing the efficiency of small interfering RNA (siRNA) loading into callus-derived vesicles using various techniques, including sonication, incubation, incubation with saponin, lipofection, and electroporation. We observed significant differences in loading efficiency and yields among the different sources.

Additionally, pEXs were isolated from tobacco callus and suspension cultures, as well as apoplastic fluid, and loaded with the anti-cancer drug doxorubicin (DOX). These loaded exosomes successfully entered rat mesenchymal stem cells (rMSC) and tobacco cells, demonstrating their capacity to deliver therapeutic agents. Moreover, molecular characterization identified the exosomal marker HSP70 and the secondary metabolites nicotine and anabasine in the vesicles.

Our findings highlight the potential of plant-derived pEXs as natural nanocarriers for drug delivery, leveraging their intrinsic bioactive compounds and optimizing production and functionalization for enhanced therapeutic applications.

Research highlights

1) Comparative analysis of pEV yields from apoplastic fluid, sterile calli, and suspension cultures.
2) Assessment of siRNA loading efficiency into callus-derived vesicles using various techniques.
3) Molecular characterization identified HSP70, nicotine, and anabasine in tobacco-derived vesicles.
4) Effective loading with anti-cancer drug and delivery of loaded pEXs into rat mesenchymal stem cells (rMSC) and tobacco cells

# Talks session 4
# (TU 9:30 – 10:50)

# Molecular modeling of alkali halides using phase-transferable models: aqueous solutions, anhydrous crystals, crystalline hydrates, molten salts

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Electrolytes, particularly alkali metal halides, are essential in both biological functions and various industrial applications. Understanding their microscopic behaviour is crucial for optimizing their use in areas such as energy storage and nuclear power. This research uses classical molecular simulations with phase-transferable polarizable models developed in our group [1] to study the microscopic nature and thermodynamic properties of alkali metal halides in various phases, including aqueous solutions, anhydrous crystals, crystalline hydrates, and molten salts.

1. We have performed a comprehensive study of alkali metal halide hydrates [2], filling a gap in previous research that has often neglected crystalline hydrates, with the exception of NaCl⊕2H2O. Our results show that while non-polarizable force fields have limitations in modeling hydrates containing Li+ cations, polarizable force fields show better accuracy, with the exception of LiCl⊕H2O. 2. We have studied the structure of concentrated alkali metal halide solutions [3] and explained the aqueous solution structure based on three imaginary driving forces. The results show and quantify how the strengths of the hydration bonds of different ions vary and how the hydration numbers decrease with increasing concentration in parallel with an increase in the number of contact cation-anion pairs. 3. We study the concentration dependence of aqueous salt solutions at low temperatures in the range of maximum density. The predictions of the polarizable models are comparable to the selected non-polarizable models and their deviations from experiments are rather due to the inaccuracy of the water models used. 4. We study different caesium halide crystal structures and show that our force fields predict their stability and structure well. 5. We study the thermochemical properties of anhydrous crystals and molten salts at high temperatures.

Research highlights

1) Calculation of crystal lattice parameters for crystalline hydrates.
2) Structure of concentrated alkali metal halide solutions.
3) Aqueous salt solutions at low temperatures.
4) Structure of caesium halide crystals.
5) Anhydrous crystals and melts at high temperature.

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# Biochar Assisted Phytoremediation with *Miscanthus × giganteus* in Trace Elements Contaminated Soil

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*Miscanthus × giganteus (Mxg),* a perennial rhizomatous grass with C4 photosynthesis, is effective for phytoremediation of post-mining soils contaminated by trace elements (TEs) [1]. Biochar, produced through slow pyrolysis of biomass, is a soil amendment that enhances soil fertility and health, supports phytoremediation, and boosts plant biomass productivity [2].

This study had a goal to assess the phytoremediation potential of *Mxg* toward TEs contaminated soil from post-coal mine in Vrsebořice when the process was supported by biochar. Two biochars produced, consequently, from the food & wood wastes (FWB) and sewage sludge (SSB) were researched in two doses: 3.5% and 7%. FWB had pH of 9.87, SBET of 10.7 $m^2/g$, 62.4% porosity, and high content of Zn. SSB had pH of 9.34, SBET of 17.4 $m^2/g$, 51.7% porosity, and high content of Al, Fe, Ca, P. The experiment was provided in a semi-field condition throught 154 days (May 5 – October 5, 2024), and the morphological and physiological parameters of *Mxg* were evaluated during the vegetation. At harvest the value of dry biomass weight (separately for leave and stems) were measured along with concentration of TEs in the different plant's tissues. The plant stress was measured along the vegetation as well. .

The results showed that SSB 7% significantly increased plant height, leaf and stem dry weight (DW), while FWB 7% increased stem DW. Both biochars at 3.5% had no significant impact on plant's bioparameters compared to the control. Fv/Fm values which indicated plant stress, peaked in August (0.78–0.80), with the highest value for control and the lowest for SSB 7%. Stress signs were least in FWB in September. Biochars at both doses reduced Cu uptake by *Mxg* compared to the control, while SSB 7% also reduced Zn uptake. Both biochars increased P and K uptake by the plant. Results indicated that the higher dose of SSB positively influenced to *Mxg* development and phyhtoremediation of TEs in soil, while smaller dose of 3.5% did not have any effect.

Research highlights

1) Incorporaion of SSB 7% enhanced *Mxg* growth parameters
2) Tested biochars reduced the uptake of Cu, SSB 7% decreased Zn uptake
3) Biochar incorporation increased the uptake of P and K by *Mxg*

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# Chitosan/alginate biofilms with deep eutectic solvents in Microbial Fuel Cells

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The significant increase in global energy consumption and the high cost of electricity in recent years have led to a worldwide energy crisis. Currently, over 80% of the world's primary energy supply comes from non-renewable sources, such as fossil fuels. Studies indicate that natural resources like coal may be depleted within a century, with oil reserves potentially running out even sooner . As a result, researchers are increasingly focusing on developing alternative technologies for bioenergy production. Among the most important advancements in this field are microbial fuel cells (MFCs), which can generate electricity from a wide variety of waste materials, including domestic and industrial wastewater [1]. MFCs are an emerging technology that simultaneously treats wastewater and recovers energy. These devices use microbial metabolism to generate electricity from organic matter. A key component in the design of MFCs is the separator, which is essential for transporting protons from the anode to the cathode and has a significant impact on the performance of the cell [2].

The membranes were characterized in a two electrode configuration in order to know the internal resistance of the membranes. Internal resistance values were calculated from Nyquist plots, which in turns were obtained with the AC Impedance Spectroscopy method, FRA (frequency response analysis) (Autolab PGSTAT302N, Metrohm Autolab B.V., Utrech, The Netherlands). Membranes were also characterized using a scanning electron microscope (SEM) and VegaTC software and Fourier-transform infrared spectroscopy (FTIR).

Research highlights

1) New membranes were prepared by using the biopolymers such as chitosan and alginate
2) Deep eutectic solvents were used as a filler into these membranes
3) These new composites can be used as a separators in MFCs.

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# Computational Fluid Dynamics Studies for Optimizing Stem Cells Cultivation

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Stem cells offer promising avenues for the treatment of a wide range of diseases, particularly cancer and heart disease. The development of new therapies using these cells is currently hampered in part by the limited quantities in which they can be isolated from tissue [1]. Studies show that cultivation in a mixed-suspension bioreactor yields better results than conventional 2D cultures. To improve this process, computational fluid dynamics (CFD) studies have been instrumental in optimizing the bioreactor environment.

The goal of this research is to optimize the cultivation process in a bioreactor by achieving a homogeneous suspension and ensuring a cell-friendly environment, i.e., the cells are constantly in buoyancy and not subjected to high shear stress over a long period of time. The current study focuses on CFD modeling and presents basic numerical simulations of fluid mixing dynamics in a stirred bioreactor. Two software packages, OpenFOAM and Ansys CFX, governed by the continuity and Navier-Stokes equations, were used.

Our research employed the Moving Reference Frame (MRF) and Arbitrary Mesh Interface (AMI) methods to model the rotating components and interactions within the bioreactor precisely. To ensure the accuracy of our results, we conducted Particle Image Velocimetry (PIV) experimental measurements to validate the CFD data. For further verification, we evaluated velocity profiles in three horizontal and two vertical planes using MATLAB software. Following this rigorous verification process, we conducted a parametric study to investigate the effects of stirrer speed, stirrer length, and stirrer diameter on bioreactor performance. The results highlight the significant impact of these parameters on the efficiency of stem cell cultivation and provide insights for optimizing industrial bioreactor designs to improve cell yield and viability.

**Research highlights**

- CFD studies are used to optimize the bioreactor environment.
- PIV measurements are used to validate CFD data.
- Effects of stirrer speed, length, and diameter are investigated.

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**Acknowledgements:** This research is supported by the Internal Grant Agency of Jan Evangelista Purkyně University in Ústí nad Labem (project no. UJEP-SGS-2023-53-005-3).

# Talks session 5
# (TU 11:20 – 12:40)

# Assessment of Biochars Properties Prepared from Different Feedstocks and Their Prospects as Carbon-capturing and Sequestering Construction Materials

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Manufacturing of cement has become a global threat due its contribution to greenhouse gas emissions. About 7% of global carbon dioxide is released through different stages of cement production [1]. Using biochar in concrete industries to absorb atmospheric carbon dioxide is a sustainable solution of the problem [2]. It is predicted that biochar can be helpful to reduce approximately 1.5% of total annual global CO2 emission if only 373 million tonnes of biochar are produced from agricultural waste per year [3]. The main objective of the study was to characterize different biochars and assess the strength and carbon capture potential when added to construction materials. Two different types of biochars were studied from food-wood waste (FWB) and sewage sludge (SSB) feedstocks. Both biochars are alkaline in nature, FWB had porosity about 62.5% and SSB had a porosity of 51.7%. Specific area of SSB (17.5 $m^2$/g) was higher than FWB (10.7 $m^2$/g). Results from the ultimate analysis revealed that FWB had higher content of carbon (73%) compared to SSB, whilst, SSB had much higher content of oxygen (62.5%). Additionally, SSB was more volatile, because of its less water content. Biochar samples were added to cement mortar at three different doses of 2 wt%, 4 wt% and 8 wt%. The results showed that 2 wt% of SSB had 6% higher flexural strength than control mortars in a 7 day test, whilst, there was no significant impact of FWB. A similar trend was observed for a 28 day test. The compressive strength was improved considerably on the 28 day test for SSB 2 wt%, though it was less in the 7 day test smaller compared to the control specimens. Analysis for the carbon adsorbtion by biochar amended construction materials are currently ongoing.

## Research highlights

1) FWB contained higher carbon, while SSB had more oxygen content.
2) No considerable influence of FWB doses in the cement mortars.
3) Addition of SSB 2 wt% increased flexural and compressive strength of mortars.

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# Modification of graphene-like materials and polymer thin films with energetic ions for their application in energy storage

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The positive impact of ion implantation on modifying the electrical properties of polymers has been known for a long time [1]. This process induces chemical and physical changes, altering the internal structure of polymers through the formation of free radicals, reorganization of molecular chains, and the creation of new chemical functional groups, which subsequently affects their mechanical and electrical properties [2,3]. This method offers a promising alternative to produce new electronic components without the need for pure metals. Based on our laboratory studies on multi-energy ion implantation of Au ions, we decided to further investigate this technology [4].

The initial research focused on the implantation of energetic $Cu^+$ ions into graphene oxide (GO) and polyimide (PI) at an energy of 1500 keV with ion fluences of [$3.75x10^{12}$, $3.75x10^{14}$, $1x10^{16}$] ions/cm$^2$ and their impact on the change of electrical properties of the modified materials [5]. In this work, the changes in sheet resistance were measured using the two-point method in a vacuum atmosphere. The measurements confirmed a significant change in sheet resistance, especially in the case of PI, with an increase of nearly 11 orders of magnitude. Additionally, humidity sensor testing of both materials was conducted, where modified GO showed a significant change in sheet resistance with increasing humidity.

Following this research, additional materials were selected for their potential application in electronics, sensing, or direct electrical energy storage, based on their altered electrical properties. This time, thin layers of graphene (G), polyimide (PI), polymethyl methacrylate (PMMA), and cyclic olefin copolymer (COC) were implanted with multi-energy [2.8, 2.0, 1.8] MeV $Cu^+$ and $Ag^+$ ions with ion fluences of [$1x10^{12}$, $1x10^{13}$, $1x10^{14}$] ions/cm$^2$. In this study, electrical properties were tested not only under direct current but also under alternating current using the newly applied technique of electrochemical impedance spectroscopy (EIS). This technique revealed interesting findings, particularly regarding the electrical properties of graphene, which, after implantation, showed promise for use as anodes in lithium batteries. The disrupted structure of graphene resulted in reduced electrical conductivity, leading to a slight increase in its resistivity without damaging the structure to the extent that electrical conductivity would be interrupted. This fact can be highly desirable for increasing the electrical capacity of graphene, which is advantageous for its use as an anode in lithium batteries.

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# Harnessing Perfluorocarbon-Based Nanocarriers for Rhodium (III) NHC Complex Delivery: Synthesis, Characterization, and Cytotoxicity Evaluation

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The optimisation of drug delivery systems is essential for improving therapeutic efficacy, particularly for drugs with low water solubility. Nano-based drug delivery systems offer promising solutions, utilizing nanoparticles (NPs) and nanocapsules to enhance the solubility, stability, targeting, and controlled release of drugs. Novel rhodium (III) complexes with an N-heterocyclic imidazolidene carbene-bearing polyfluoralkyl tag were synthesized, followed by their encapsulation in albumin-derived perfluorcarbon-based nanocapsules. The characterization of the synthesized complexes using various techniques such as NMR spectroscopy, mass spectrometry etc. confirmed the successful formation of the complexes. The fluorophilicity of the complexes, crucial for the preparation of perfluordecalin-filled nanocapsules, was determined through the evaluation of their partition coefficient, indicating their affinity for fluorinated environments and their suitability for incorporation into perfluorocarbon-based nanocarriers. The resulting nanoemulsions containing these complexes displayed small droplet sizes and negative zeta potentials, indicating physical stability. Furthermore, the minimal changes in particle size distribution of the capsules after three weeks storage suggest their potential long-term stability. EDX analysis confirmed the presence of rhodium within the capsules. These findings highlight the potential of perfluorocarbon-based nanocarriers for effective drug delivery.

Research highlights

1) Synthesis of novel rhodium (III) complexes with N-heterocyclic imidazolidine carbene bearing polyfluoralkyl tag.
2) Evaluation of fluorophilicity through partition coefficient, indicating affinity for perfluorinated environments.
3) Characterization and long-term stability of resulting PFD-filled nanocapsule, showcasing potential for effective drug delivery.

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# Influence of $CeO_2$ nanoparticles and alginite particles on microbial communities in hemp rhizosphere and soil: DNA sequencing and bioinformatics approach

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Recent advances in nanotechnology have introduced novel agricultural applications, raising questions about their impact on soil ecosystems. This study investigates the influence of cerium oxide nanoparticles and alginite particles (both micro- and nano-sized) on the microbial communities associated with the rhizosphere and soil of hemp (*Cannabis sativa L.*), with a focus on assessing potential harm to microbial growth and diversity. Hemp plants were cultivated under controlled greenhouse conditions for three weeks. Microbial community dynamics were assessed through DNA extraction from root and soil samples, followed by next-generation sequencing (NGS) utilizing the Illumina platform. Comprehensive bioinformatics analyses were conducted to elucidate the composition and functional potential of the microbial consortia. The findings demonstrate alterations in microbial populations induced by the particle treatments, providing detailed insights into the effects of nanomaterials on plant-microbe interactions. This research underscores the importance of evaluating nanotechnology's impact on rhizosphere microbiomes to ensure sustainable agricultural practices and soil health.

Research highlights:

1) Cerium oxide and alginite particles influenced the microbial communities in hemp rhizosphere and soil, while overall diversity showed resilience.
2) Morphological measurements indicated no significant detriment to plant habitus development.

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# Posters session
# (MO 16:00 – 18:00)

# Distinguishing of anthropogenic contamination and natural geogenic anomaly in soils in Northwestern Bohemia

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Many historical industrial activities, including coal mining and burning, began near geogenic anomalies. The result was a spatial overlap of anthropogenic and natural causes of increased contents of soil risk elements. Conventional geochemical soil mapping cannot distinguish anthropogenic and geogenic contributions here, especially when only pseudo-total contents of risk elements were obtained, soil depth profiles were not taken, and geological maps were not implemented.

Local geology, topography and anthropogenic activities were taken into account when planning soil sampling. Soil profiles were obtained using an auger sampler. Total contents of hazardous and lithogenic elements were obtained by X-ray fluorescence. Aqua regia extraction and inductively coupled plasma mass spectrometry (ICP-MS) were also used for analyses. PAHs were analyzed by GC-MS.

Coal use in the study area increased soil Cd, Hg, Zn, and PAHs within a radius of max. 10 km east of the large power plant. The highest contents of As and Pb in the soils of the Mostecka Basin were caused by local geogenic anomalies and not by coal combustion.

Conventional soil mapping projects and data mining procedures cannot unambiguously decipher the anthropogenic contribution to soil risk elements, as demonstrated in this paper. When working in geogenically anomalous areas, a basic knowledge of the mechanisms controlling the content of risk elements in soils is necessary.

Research highlights

1) In locations with geogenic anomalies, detailed sampling and holistic data acquisition must be used.
2) Coal use in the study area increased soil Cd, Hg, Zn, and PAHs within a radius of max. 10 km of the power plant.
3) The highest contents of As and Pb in the soils of the Mostecka Basin were caused by local geogenic anomalies and not by coal combustion.

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# The Effect of Ryegrass on Enhancing Soil Carbon and Nutrients Storage

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The study explores the enhancement of soil parameters, cycle of nutrients, and soil quality, including soil physical and biological parameters. The ryegrass is used commonly as a cover crop and can improve quality of soil given that its extensive root system supports nutrient uptake inclusive of N, P and K. In addition, biomass formed aboveground would increase soil organic matter while decomposition occurs increasing C content (Finn et al., 2013).

A pot experiment was conducted in a greenhouse with Italian Ryegrass (IG) and Perennial Ryegrass (RG) to compare the effects of these plants on soil organic carbon and nutrient cycle including total organic carbon (TOC), total nitrogen (TN), total sulfur (TS), and total phosphorus (TP). Moreover, the study examines microbial biomass dynamics revealing the impact of Italian and Perennial ryegrass on soil microbial communities and emphasizing the crucial role of plant-microbe interactions. For a better holistic approach, the soil enzymatic activities involved in the cycle of elements was studied. The values before and after planting were reviewed for all the studied parameters.

This research emphasizes the importance of considering plant species selection in agricultural systems, as it can significantly influence soil health, fertility, and ecosystem functioning. By promoting the cultivation of Italian Ryegrass (IG) and Perennial Ryegrass (RG), and implementing sustainable management practices, it is possible to enhance soil carbon sequestration, improve nutrient cycling, and contribute to the long-term sustainability of agroecosystems.

Research highlights

1) Finding indicates the influence of vegetation type and environmental factors on TOC levels, with IG exhibiting the higher TOC content of 24.84 ± 0.90 g/kg (22% higher than RG).
2) Results showed significant increase in IG across the enzymatic activities in the greenhouse setting with 1.9 %, 77 %, and 3.7 % increase in phosphatase, protease, and arylsulphatase respectively.

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# Birch foliar analysis for mapping weak soil contamination by zinc

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This study builds on a previous one, where birch (*Betula*) leaves were shown to be of interest for monitoring soil contamination with zinc [1]. Biomonitoring can serve to evaluate real risks related to the chemical contamination of soils, as it characterises the actual entry of risk elements into biotic cycles and, thus, the actual impact of contamination on organisms in a more straightforward manner than that of chemical proxies for contaminant bioavailability. However, biota are not direct sampling probes that respond linearly to soil contamination. Deciphering the patterns underlying the uptake of risk elements by plants presents a challenge.

Zinc is a risk element that has been anthropogenically elevated in environment for centuries. Zn is an essential element for plants and is not toxic unless present in extreme amounts.Foliar Zn from two birch species, *Betula pendula* and *B. pubescens*, that are common in temperate and boreal European forests was analysed in several case studies in two districts of the Czech Republic and the southwestern Finland. Leaf and soil samples were collected from the Czech Republic, while in Finland only leaves were sampled. The Finnish collection was also analysed using a handheld X-ray fluorescence spectrometer to assess if the non-destructive analysis of fresh leaves can be used for field mapping. Typical foliar Zn concentrations in uncontaminated areas were present in the three main populations centred at approximately 100, 160, and 260 mg $kg^{-1}$, depending on the geographic setting. Birch foliar Zn concentrations are elevated in areas impacted by coke, iron, and steel manufacturing in Třinec, Czech Republic, around the power plant in Naantali, south west Finland (foliar Zn ca. 400 mg $kg^{-1}$ in both cases), and also within a 10 m belt around transportation routes in northern edge of Ústí nad Labem, Czech Republic (foliar Zn ca. 300 mg $kg^{-1}$).

The advantage of using birch foliar Zn concentration for contamination mapping instead of using soil samples is that foliage directly characterises Zn uptake by biota, even in complex terrains such as mountain forest soils and anthropogenically impacted terrains where the depth of representative soil sampling is questionable.

Research highlights

a Birch leaves are suitable for mapping soil contamination by zinc
b Handheld X-ray fluorescence spectrometer can be used for fresh leaves in field
c Zinc emissions from energy, iron, and steel production and cars and railroads were mapped

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# The effect of acidifying pollution on spruce growth

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From the 1970s to the 1990s, acidifying pollution caused significant mortality and growth reduction in spruce trees across Europe, particularly in the "black triangle" – a region encompassing the northern Czech Republic and the border areas of Germany and Poland. However, the extent of pollution varied within this region. Our recently published study [1] explores why spruce tree growth in the Ore Mountains (Krušné hory) and the Giant Mountains (Krkonoše) exhibited similar reductions despite the latter being less polluted.

We collected and analysed tree-ring width data for Norway spruce (*Picea abies* [L.] Karst) from both Czech regions and compared them to data from neighbouring countries. We then examined the correlations between tree-ring widths and historical pollution according to the EMEP MSC-W model [2]. Our findings indicate that atmospheric sulfur deposition negatively affected tree-ring width up to a threshold, beyond which further increases in sulfur deposition did not result in additional growth reduction. This could explain why we observed a similar ring-width reduction in spruce from the Ore Mountains and the Giant Mountains. This suggests that trees experiencing a higher growth reduction may have died and were thus not sampled. Furthermore, low quantities of oxidised nitrogen deposition seemed to have a positive impact on tree-ring width, possibly due to a fertilising effect.

Our sampled trees in the Ore Mountains and the Giant Mountains showed comparable recovery in growth following the decline in air pollution in the 1990s. While liming affected soil characteristics, it did not seem to influence spruce growth recovery. This supports the findings of other studies [3,4] that air pollution, combined with extreme weather conditions, was the main factor limiting tree growth.

Research highlights

1) Acidification reduced spruce growth across the black triangle in 1970–1990.
2) Spruce outside the black triangle was significantly less affected.
3) Spruce growth was found to be mainly affected by sulphur dioxide in the air.
4) Liming did not seem to greatly improve the recovery of the spruce trees.

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# External electric field induced structural change of oligo(ethylene glycol) in explicit solvents: A molecular dynamics study

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Polymer materials exhibit microscopic structural changes when subjected to an electric field, which is significant for a wide range of applications, including electrospinning technology [1]. In this study, we investigate the structural properties of oligo(ethylene glycol) with varying chain lengths in water and methanol under an external electric field using extensive molecular dynamics simulations. These simulations were performed to elucidate the results of our previous study [2]. We analyze the size and shape anisotropy of the oligomer chain using the end-to-end distance, radius of gyration, and metrics derived from the gyration tensor. We calculate the distributions of dihedral angles, the cosine of the angles of the monomer units, and the dipole moments of the chain and solvents relative to the direction of the electric field. To quantify the helicity of the chain, we count the monomer units predefined helical patterns. Our results show that the initially isotropic chain in both solvents becomes increasingly anisotropic and adopts an oblate shape as the field intensity increases. However, this effect diminishes with increasing chain length in water. The population of the gauche conformation increases significantly as the field intensity increases. In methanol, the monomer units of the chain align perpendicular to the field, whereas in water, there is a deviation towards smaller angles. Additionally, the dipole moments of both the chain and solvents progressively align with the field direction.

Research highlights

1) Carry out molecular dynamics simulations of ethylene glycol oligomers in polar solvents.
2) Identify changes in the structure of an oligomer molecule caused by an electric field.
3) Describe how the changes observed are influenced by both the intensity of the electrostatic field and the length of the oligomer chain.

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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# Effect of variety on the chemical composition of the grain of spelt (Triticum. spelta L.) wheat

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Spelt (Triticum spelta) is a hexaploid wheat with a hulled grain and a brittle rachis, known for its valuable agronomic properties. Spelt grain is more abundant in iron, zinc, copper, magnesium, potassium, sodium and selenium than bread wheat. Compared to wheat, spelt has a higher protein and lipids contents, but lower insoluble fiber and total fiber contents. It also contains more proteins, mineral elements, lipids, fiber, and vitamins than bread wheat and possesses a more suitable composition of amino acids. This study aims to evaluate the effect of five macro- and fifteen microelements risk elements in the, spelt wheat cultivars, all grown under field conditions. All elements were determined by ICP-MS analysis. The chemical composition of spelt wheat in the field area and quantitative analysis of major components in spelt wheat grains, including moisture, protein, fat, carbohydrate, fiber, and ash contents respectively. Identification and quantification of specific nutrients, such as vitamins and minerals. Further work will display the analysis of varietal differences and specific genes associated with different chemical traits in the chemical composition of spelt wheat grains. The following grain parameters will be tested: Total protein content – Total Ash content- Crude Fat-Starch- Lipid- Dietary fiber and contents of macro-micro elements, basic nutrients in grain, milling quality of grain, and bread quality, grain yield, plant height, phenological stages.

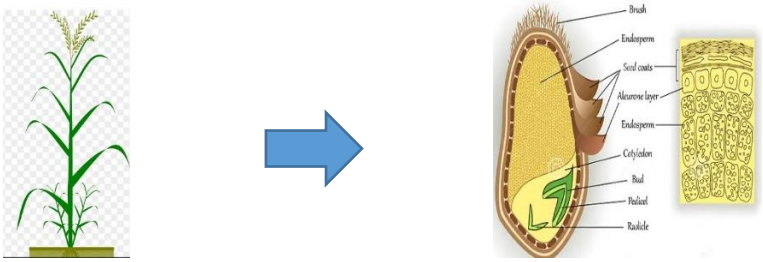


**Fig 1. Spelt wheat Taxonomy.**

*Research highlights*

- My study will investigate the morphological traits of different spelt wheat varieties connected with the chemical composition of the grain
- My study will determine content of micro, macro and risk elements in grain of different varieties with respect to the nutritional value of the grain
- My study will compare the content of macro elements and micro elements in the grain of T. spelta hybrids and also crossbreeding could contribute to improving the nutritional quality of wheat

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# Liquid exfoliantion of molybdenum disulfide for hydrogen evolution reaction

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This project aims to exfoliate bulk molybdenum disulfide ($MoS_2$) powders using solvent-assisted sonication, targeting their application in the hydrogen evolution reaction (HER). Two $MoS_2$ powders with different particle sizes were used: one with particles smaller than 2 micrometers and the other with particles smaller than 6 micrometers. The exfoliation process was optimized by experimenting with various solvent mixtures, which resulted in the identification of two potentially ideal solvent combinations.

Exfoliation experiments involved preparing two sample series with 5 ratios of the two selected solvents mixtures. Exfoliated samples were characterized using techniques such as Atomic Force Microscopy (AFM), Dynamic Light Scattering (DLS), Scanning Electron Microscopy (SEM), Raman Spectroscopy, X-ray Diffraction (XRD), specific surface area measurements, and electrochemical property analysis.

Preliminary results from Raman spectroscopy indicate successful exfoliation, evidenced by a specific shift between the characteristic peaks of $MoS_2$. The ongoing analysis will provide additional insights into the structural and electrochemical properties of the exfoliated $MoS_2$, contributing to the development of efficient catalysts for hydrogen evolution reactions.

Research highlights

1) Optimization of solvent mixtures and exfoliation conditions.
2) Preliminary results from Raman spectroscopy indicated successful exfoliation.
3) Some samples perform better in HER than bulk powder.

# Variability of durum wheat (*Triticum durum*) in intake and accumulation of zinc

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Malnutrition due to lack of zinc intake is a worldwide problem. It is most pronounced especially in developing countries, but it is also relevant for developed countries. Plants also need zinc in the right amount, because it is involved in various physiological functions and enzyme activities, including the production of proteins and auxins, glucose metabolism, building the immune system and the proper function of cell membranes. Low levels of micronutrients in plants are related to their decreasing concentration in the soil or their low bioavailability and abiotic stress, which disturbs the proper growth and development of plants. The lack of zinc for plants causes a reduced yield of cereals and thus certain socio-economic impacts. A possible solution with demonstrably positive results is the agronomic biofortification of wheat. We analyze a set of 13 varieties of durum wheat (Triticum durum) for Zn tolerance and Zn accumulation in grains. By conventional laboratory procedures of molecular biology, phenotyping and analytical chemistry, we select varieties suitable for biofortification programs. We will compare the mechanisms that could be responsible for the observed differences, such as the accumulation of metabolites or the activity of genes for the production of phytochelatins. The goal of the research is also to evaluate the effect of arbuscular mycorrhizal fungi (AMF) on the uptake and accumulation of Zn in the grains of the tested varieties. We are currently analyzing the data from the phenotyping of the experimental material, while evaluating the effect of AMF, soil application of Zn and their combination on the growth, development and photosynthetic parameters of plants. Preliminary results confirm intraspecific variability in Zn tolerance and the effect of mycorrhizal fungi.

Research highlights

1) Clarification of income mechanisms and of zinc transport in plants and the selection of wheat varieties that will become the starting point for the breeding of varieties for organic cultivation.
2) Potential use of the wheat gene pool in solving the problem malnutrition in healthcare or food industry

Acknowledgment: The paper was supported by the Research and Development Agency under grant no. APVV-21-0504.

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# A perfusion system for testing of the effects of electrical field on osteogenic differentiation of human mesenchymal stem cells

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Bone tissue engineering has emerged as a promising alternative to traditional bone grafts, primarily because of the limitless availability of the engineered tissue and absence of disease transmission risks. Despite its potential, it has yet to be fully integrated into clinical practice due to various limitations and challenges. Bone formation in the body is a complex and highly regulated process, influenced by numerous biochemical and physical factors. To effectively create a bone tissue engineering construct, it is essential to consider and integrate all these components to achieve in vivo-like stimulation of target cells.

Electrical stimulation has been identified as a promising technique in bone tissue engineering, known to enhance vital cellular processes such as proliferation, migration, and differentiation. In our research, we are developing a perfusion system that allows for convenient observation of the effects of electrical field stimulation, alongside other factors like oxygen levels and substrate properties, on the behavior of human mesenchymal stem cells (HMSCs).

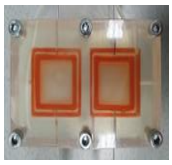

**Figure 1** assembled system prototype

Research highlights (still in development)

1) Designed and manufactured a prototype of perfusion system for testing of the effects electrical field on human mesenchymal stem cells.
2) Human mesenchymal stem cells show different migration directionality under the effect of alternating electrical current.

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# Temporal Trends in Winter Wheat Yields: The Role of Fertilization, Proceeding Crop and Weather Over Decades of Field Experiments

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Climate change is undoubtedly one of the most important factors affecting agricultural production. The characterization of adverse weather and the quantification of their potential impact on arable farming is necessary to advise farmers on feasible and effective strategies. The primary aim of our research was to assess the interactions between differentiated fertilization management and environmental factors, examine their influence on wheat yield and varietal response with time, minimize nitrogen (N) fertilizer using Alfalfa as a proceeding crop, and recommend an appropriate N dosage based on the latest scenarios. A long-term experiment including 15 seasons (1961-2022) was analyzed, where a wheat crop followed alfalfa as a proceeding crop was cultivated with different N treatments. We found that the average temperature in the Caslav region has increased by 0.045°C per year, more significantly since 1987. Additionally, precipitation slightly decreased by -0.247 mm, but not significantly. Wheat yields were more sensitive to temperature than precipitation changes. The average November temperatures are gradually rising, positively affecting wheat grain yields. July precipitation negatively impacts grain yields only in years with extraordinary rainfall. The application of higher doses did not lead to a significant grain yield increase. Alfalfa, as a preceding crop, reduced the need for N fertilization and contributed to sustainable conventional agriculture. Further, new wheat varieties (Contra, Mulan, Julie) yielded statistically more than the old variety (Slavia). Properly managing N in different climate scenarios is crucial for enhancing plant growth while minimizing N environmental losses. In conclusion, the optimal N dosage was determined at 65 kg ha$^{-1}$ N, corresponding with the average yield of 9.1 t ha$^{-1}$ following alfalfa as a proceeding crop.

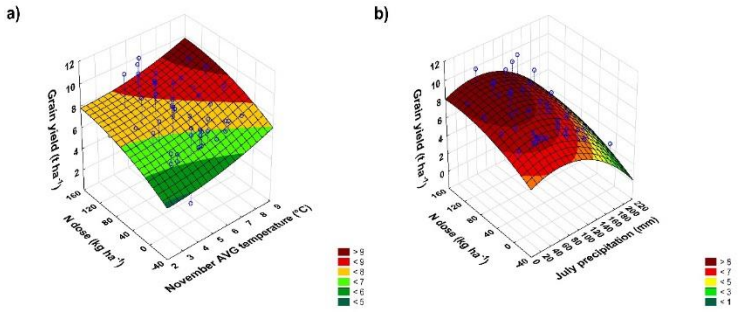


**Figure 1**. The relationships between grain yield (t ha$^{-1}$), N dose (kg ha$^{-1}$), and a) average temperature in November (°C), and b) sum of precipitation (mm) in July. The colour scales (right corners) represent the yield rate (t ha$^{-1}$) of winter wheat.

**Research highlights**

1) Temprature in Caslav region is gradually Increasing
2) Alfalfa cultivation as a proceeding crop can minimize nitrogen expense
3) New varities responded in better yield acomparively with old varities in changing climate

# 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] Last year it was 100 years since the first separation of $Li_2CO_3$ from the zinnwaldite mineral mined for Cínovec. In 1923, the German company Metallgesellschaff - Frankfurt/Main introduced the production of lithium salts and lithium metal at the Hans Heimich Hütte Langlesheim. At first it processed amblygonite, later it switched to processing zinnwaldite from the Cínovec deposit in the Krušné hory.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 $Ca(OH)_2$. Three fusion mixtures were created with different ingredient ratios. 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. According to the amount of lithium transferred into the solution, the ideal temperature and time of leaching for each mixture was determined. 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

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# Microfluidic Blood-Brain-Barrier model for extracellular vesicles transport studies

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One of the greatest obstacles for effective cancer treatment are blood-tissue barriers. Their purpose lies in protecting tissues and organs from adverse factors present in blood streams by strict control of their transport. Effectiveness of newly designed drugs thus depends on their ability to pass through the blood-tissue barriers in sufficient concentrations[1]. One of the promising drugs and drug carriers (vectors) are extracellular vesicles – exosomes[2]. Exosomes are a sub-micron secretion products of mammalian, animal and plant cells with great biocompatibility (biological origin).

This work is focused on fabrication of microfluidic lab-on-chip device [3] to simulate blood-brain barrier (BBB) in laboratory conditions and on study of transport mechanisms of extracellular vesicles (exosomes).

Experimental BBB microfluidic model was built in previous work. Vertically organized glass device with inserted perforated polycarbonate membrane was successfully tested as BBB model with possibility to perform transport studies. To extend our abilities for optical verification of cultivated cells and quantification of effectivity of the exosome transport, we opted to fabricate BBB models in parallel channels with perforated walls between them. To achieve reliable BBB models, COC (cyclic olefin copolymer) and FlexDym (SEBS) were chosen as suitable materials in combination with fabrication by hot embossing.

Research highlights

1) Succesfull cell cultivation (endothelium) in glass and in FlexDym-glass microfluidic devices.
2) Blood-brain barrier formation in vertical glass microfluidic device.
3) Optimized fabrication processes for devices from glass, COC and FlexDym materials.

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# *Miscanthus x giganteus*: An Industrial Crop for Phytoremediation of Pharmaceuticals from Hospital Wastewater in Soil

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**Presenting author, e-mail: zubairuaf1@gmail.com 1st year of PhD, study program: Landscape reclamation and ecosystemservices*

*Miscanthus* × *giganteus* is a perennial rhizomatous grass with $C_4$ photosynthesis, notable for its ability to withstand cold temperatures while maintaining an adequate photosynthesis rate. It has emerged as a promising industrial crop for phytoremediating soils contaminated by trace elements and pharmaceuticals, providing dual benefits of biomass production for energy and environmental improvement (Pidlisnyuk *et al*., 2021). This study aims to evaluate the phytoremediation potential of *Miscanthus* × *giganteus* in soils contaminated with pharmaceutical active compounds typically found in hospital wastewater (HWW). The pharmaceuticals under investigation include Carbamazepine, Clarithromycin, Ketoprofen, N-acetylsulfamethoxazole (metabolite), Pentoxifylline, Estrone, Phenazon, Diclofenac, Tramadol, and Venlafaxine (Carter *et al.,* 2015) These contaminants pose significant risks to soil health, human health, and the environment. The study involves applying different concentrations of HWW to soil in pots planted with *Miscanthus* × *giganteus* and in unplanted control pots. A comprehensive set of physio-chemical and biological parameters will be measured to assess the remediation efficiency and impact on soil and plant health. The parameters include pH, total suspended solids (TSS), chemical oxygen demand (COD), biological oxygen demand (BOD), electrical conductivity (EC), bio concentration factor (BCF), translocation factor (TLF), soil organic carbon (SOC), available phosphorus, total $CaCO_3$, cation exchange capacity, nitrogen content, microbial biomass carbon, soil basal respiration, and enzymatic activities.

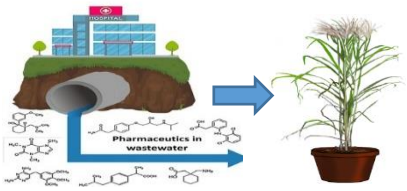


**Figure 1**

*Research highlights*

- My study will investigate the impacts of *Miscanthus* × *giganteus* cultivation on soil with different concentrations of HWW by examining various soil agronomic, physio-chemical, and biological indicators of soil health.
- My study will evaluate the phytoremediate of Pharmaceutical active compounds (PhACs) from HWW in soil.
- My study will assess the impacts of PhACs on *Miscanthus* × *giganteus* health and stress by examining specific biomarkers.

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