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2023

Proceedings of Abstracts

INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS OF THE CAS

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Ambient organic aerosol origin at rural background site in the Czech Republic

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Introduction

Atmospheric aerosols (AA) are ubiquitous particles in the atmosphere that influence the Earth's climatic system, environmental interactions, and human health. Among AA, great interest is dedicated to organic aerosols (OA) since it can represent from 20 to 90% of total submicron mass. Source apportionment of OA at background sites is one of the important tasks of current air quality protection.[1]

Methods

The variability of OA concentrations and their origin during four measurement campaigns was studied at the rural background station National Atmospheric Observatory Košetice (NAOK) in the Czech Republic. Ambient aerosol measurements of non-refractory PM_1 (NR-PM_1) were performed using a Compact Time-of-Flight Aerosol Mass Spectrometer (C-ToF-AMS,[2]) from 8th January to 14th October 2019 with a 5-min time resolution. The C-ToF-AMS measurements were supplemented with equivalent black carbon (eBC) data using an aethalometer (Model AE33, Magee Scientific, Berkeley, CA), 1-hour boundary layer height (BLH) by satellite measurements (ERA hourly dataset provided by the Copernicus Climate Change Service), 72-h back-trajectories (GDAS 1°) for every hour using the Hybrid Single Particle Lagrangian Integrated Trajectory model (HYSPLIT) and 1-hour meteorolocigal data. 30-min averages of NR-PM_1 were calculated and Positive Matrix Factorization (PMF) with multi-linear engine (ME-2) was applied, alongside the use Source Finder (SoFi,[3]) was used.

Results and discussion

Five OA factors/sources were identified during the seasons of winter, spring and autumn: biomass burning OA (BBOA), coal combustion OA (CCOA) and more- and less-oxidized OA (MO-OOA and LO-OOA). Four OA factors/sources were identified for summer, HOA, BBOA, MO-OOA, and LO-OOA. Three of these factors represent primary sources (HOA, BBOA, and CCOA), while the other two represent secondary/oxidized factors. The concentrations of individual factors were significantly influenced by meteorological conditions. The highest concentrations of primary factors seen during were periods with low wind speed and atmospheric boundary layer height. Therefore, the largest share of primary factors (29% of total OA concentrations) was found in winter and the lowest (20%) in summer. Since the aged primary OA becomes part of OOA, the percentage of primary factors cannot be directly related to the share of these emission sources in the overall immission budget.

This work was supported within a German-Czech TRACE project funded by the GACR under grant 20-08304J and by DFG under grant 431895563, by the CZ MEYS of the grants ACTRIS-CZ LM2018122 and ACTRIS-CZ RI (CZ.02.1 .01 / 0.0 / 0.0 / 16_013 / 0001315), and European Union’s Horizon 2020 research and innovation program ACTRIS IMP (871115).

References

1. Kroll, J. H. and Seinfeld, J. H. *Atmos. Environ.* **2007**, *42* 16), 3593–3624.
2. Drewnick, F.; Hings, F.;DeCarlo, P.; Jayne, J. T.; Gonin, M.; Fuhrer, K.; Worsnop, D. R. *Aerosol Sci. Tech.* **2005**, *39*, 637–658.
3. Canonaco, F.; Crippa, M.; Slowik, J. G.; Baltensperger, U.; Prévôt, A. S. *Atmos. Meas. Tech.* **2013**, *6*, 3649–3661.

How can we best eliminate pharmaceuticals from wastewater?

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Supervisors: Doc. Ing. Petr Klusoň, DSc., Prof. Jacques Barbier Jr.
Supervising Expert: Dr. Gwendoline Lafaye

Persistent pharmaceutical occurrence in different lakes and rivers usually originates from live stocks, agriculture, aquaculture, households, and hospitals. The presence of these compounds in the ecosystems leads to fatal consequences. Pharmaceuticals can threaten microorganisms in the environment, either causing its deterioration or allowing pathogens to gain resistance against antibiotics and medical treatments.[1] These occurrences in the environment questions the ability of conventional treatment to remediate pharmaceutical wastewater.

To prevent the presence of these pharmaceuticals in the environment, membrane separation may be a good choice for water purification. Due to the adjustable parameters of the membrane process, the conditions for the treated water can be optimized.[2] Moreover, membrane modifications can overcome the limitations of the process. For example, surface grafting modification can improve membrane selectivity,[3] and bulk or material base modifications or material-base can prevent the membrane from fouling by degradation or by increasing porosity.[4] However, the membrane process generates concentrated pharmaceutical solutions which are not suitable for filtration. This concentrated solution causes more concern than the diluted one. Where there is a need need to combine the membrane process with a degradation process to treat the concentrated solution instead of the expensive incineration, the best choice to degrade concentrated solutions using catalytic wet air oxidation (CWAO). The degradation process was assessed on highly concentrated antibiotic solutions under soft conditions using a 1% Pt/CeZr catalyst. The results showed 89%, 60%, and 60% antibiotics removal during the 1^{st}, 2^{nd}, and 3^{rd} cycle, respectively. Moreover, thermal *ex-situ*s catalyst regeneration allows for a full initial activity recovery. Furthermore, the treated solutions were subjected to toxicity assessments, where the treated solution of tetracycline was revealed to be non-toxic.

To sum up, the hybrid process of combining membrane separation and CWAO has great potential for pharmaceutical wastewater treatment. While the process is efficient for pollutant removal, it also avoids any chemical utilization, recovers all implemented catalysts, and is energy efficient. The membrane-oxidation hybrid process may be the key to sustainable wastewater treatment.

References

1. Bungau, S.; Tit, D. M.; Behl, T.; Aleya, L.; Zaha, D. C., Aspects of excessive antibiotic consumption and environmental influences correlated with the occurrence of resistance to antimicrobial agents. Curr. Opin. Environ. Sci. Health **2021**, *19*, 100224.
2. Kárászová, M.; Bourassi, M.; Gaálová, J., Membrane Removal of Emerging Contaminants from Water: Which Kind of Membranes Should We Use? Membranes **2020**, *10* (11), 305.
3. Bourassi, M.; Pasichnyk, M.; Oesch, O.; Sundararajan, S.; Travnickova, T.; Soukup, K.; Kasher, R.; Gaalova, J., Glycidyl and Methyl Methacrylate UV-Grafted PDMS Membrane Modification toward Tramadol Membrane Selectivity. Membranes **2021**, *11* (10), 752.
4. (a) Gaálová, J.; Bourassi, M.; Soukup, K.; Trávníčková, T.; Bouša, D.; Sundararajan, S.; Losada, O.; Kasher, R.; Friess, K.; Sofer, Z., Modified Single-Walled Carbon Nanotube Membranes for the Elimination of Antibiotics from Water. Membranes **2021**, *11* (9), 720; (b) Bourassi, M.; Karaszova, M.; Pasichnyk, M.; Zazpe, R.; Hercikova, J.; Fila, V.; Macak, J. M.; Gaalova, J., Removal of Ibuprofen from Water by Different Types Membranes. Polymers **2021**, *13* (23), 4082.

Detailed Investigation of Human Galectins -1 and -3 by employing selectively deoxyfluorinated *N*-acetyllactosamines

Student: Ing. Martin Kurfiřt
Supervisor: Mgr. Jindřich Karban Ph. D.

Human galectins (hGals) are carbohydrate-binding proteins playing key roles in a plethora of physiological processes. They are able to modulate immune responses and neoplastic transformation processes via the molecular recognition of galactoside-containing glycans.[1] As a result, the development of their selective inhibitors has become a focus of pharmaceutical research. However, the preparation of inhibitors targeting individual hGals remains challenging as 12 hGals featuring similar substrate specifications have been identified. A deeper understanding of the differences between individual hGals could facilitate the development of galectin inhibitors, and deoxyfluorinated carbohydrates are established tools capable of providing such valuable information.[2]

This work is focused on a detailed investigation of supramolecular recognition events between human galectins -1 and -3 and monodeoxyfluorinated *N*-acetyllactosamine probes, which were previously prepared in our laboratory.[3] The recognition was studied using a combination of X-ray crystallography, isothermal titration calorimetry and several advanced NMR techniques, such as ^{19}F T2-filter, ^{1}H–^{1}H STD, ^{1}H–^{15}N CSP or ^{19}F EXSY. These techniques provided insight into the thermodynamics and kinetics of recognition and enabled us to uncover of subtle differences between both investigated galectins. Such differences could be potentially exploited in the selective targeting of individual galectins with important implications for the galectins-focused pharmaceutic industry.

Support from MEYS (Project No. LTC20052 and LTC2007 2, COST Action CA18103 INNOGLY) and Czech Science Foundation (grant no. 20-01472S) is acknowledged. The author also thanks Jesús Jiménez-Barbero (CIC bioGUNE, Bilbao, Spain), Cañada Vicinay Francisco Javier (CIB, Madrid, Spain) and Roman Hrstka (RECAMO, Brno, The Czech Republic) for sharing expertise in NMR-based molecular recognition and providing human galectins.

References

1. Dings, R. P. M.; Miller, M. C.; Griffin, R. J.; Mayo, K. H. *Int. J. Mol. Sci.* **2018**, *19*, 905–926.
2. Linclau, B; Ardá, A.; Reichard, N.; Sollogoub, M.; Unione, L.; Vincent, S. P.; Jiménez-Barbero, J. *Chem. Soc. Rev. J.* **2020**, *49*, 3863–3888.
3. Kurfiřt, M.; Dračínský, M.; Červenková Šťastná L., Cuřínová, P.; Hamala, V.; Hovorková, M.; Bojarová, P.; Karban, J. *Chem. Eur. J.* **2021**, *27*, 13040–13051.

Organoruthenium glycomimetics as selective galectin-1 inhibitors

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Supervisor: Ing. Tomáš Strašák, Ph.D.
Supervising Expert: Mgr. Jindřich Karban, Ph.D.

Galectins are a type of lectins that have the ability to bind to β-galactosides. Human galectin-1 (Gal-1) and galectin-3 (Gal-3) have been linked to tumor progression, with Gal-1 contributing to cell migration and tumor immune escape, while elevated levels of Gal-3 are associated with increased invasiveness, metastatic spreading, immunosuppression, and angiogenesis. The natural ligands of galectins include galactose, lactose, *N*-acetyllactosamine (LacNAc), as well as their glycosylated and sulfated forms. Modifications of these carbohydrate ligands can lead to the creation of glycomimetics, thus enhancing binding to galectins and can serve as potent inhibitors. A common method of modification involves replacing carbohydrate hydroxyls with an aromatic substituent, which enhances binding to galectins.

Several Gal-3 inhibitors are already in clinical trials against illnesses connected with galectin overexpression, yet selective galectin-1 inhibitors are still lacking.[1] To address this, we conducted a project in which we replaced the aromatic substituent in known galectin in-

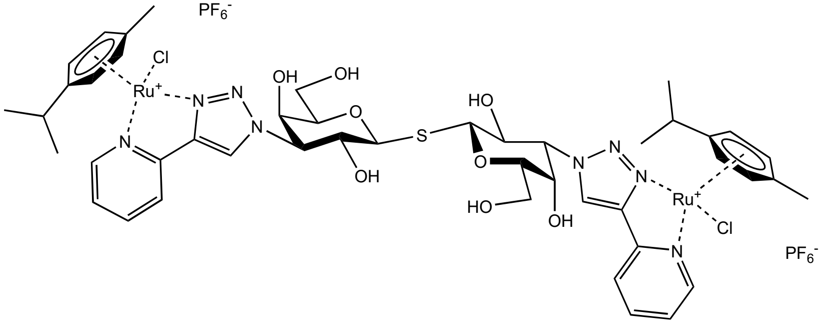

Figure 1: A structure of prepared organoruthenium highly selective galectin-1 inhibitor.

hibitors based on LacNAc, phenylthiogalactoside, and thiodigalactoside scaffolds with arene-containing ruthenium *"piano-stool"* complexes. We discovered that the unique geometry of the ruthenium ligands in these complexes creates additional favorable interactions in the binding site of Gal-1 while disrupting the inhibitor's affinity to Gal-3.

The prepared organoruthenium glycomimetics demonstrated single unit nanomolar affinity to Gal-1 and over four orders of magnitude higher selectivity to Gal-1 in comparison to Gal-3. The organoruthenium galectin inhibitors were found to be nontoxic to both cancer and noncancerous cell lines. Selected complexes showed an in vitro antimigratory effect against invasive cancer cell lines MDA-MB-231 and SK-OV-3.

This work was supported by The Czech Science Foundation (grant 23-06115S). This work was also supported by the Martina Roeselová Memorial Fellowship granted by the IOCB Tech Foundation.

References

1. Sethi, A.; Sanam, S.; Alvala, R.; Alvala, M. *Expert Opin. Ther. Pat.* **2021**, *31* (8), 709-721.
2. Kacsir, I.; Sipos, A.; Ujlaki, G.; Buglyó, P.; Somsák, L.; Bai, P.; Bokor, É. *Int. J. Mol. Sci.* **2021**, *22* (19), 10454.

Utilization of electrochemically induced cleavage of various sulfonimides

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Supervising Experts: prof. Dr. RNDr. Pavel Matějka,
prof. RNDr. Jiří Ludvík, Csc.

Currently, efforts are being made to carry out syntheses using green chemistry procedures designed (or redesigned) to reduce the environmental impacts of the processes. In this sense, the electrosynthetic approach could provide clues. Since electrochemistry brings benefits such as high selectivity in connection with facile operation, eco-friendly conditions, or economical aspects relating to lower demands for chemical agents and space, the application of this methodology is desirable. Unfortunately, the processes employing electrochemistry are still relatively rare. This could be explained by the lack of knowledge of the electrochemical redox mechanisms, which significantly differs across individual molecules due to the interplay of all functional groups present in their structures. However, the key to understanding the redox behaviour of polyfunctional molecules lies in the detailed analysis of electrochemical results at the molecular level[1]. A good example of the use of electrosynthesis was recently published by Huang et al[2], describing simple electro-reductive hydrodefunction-

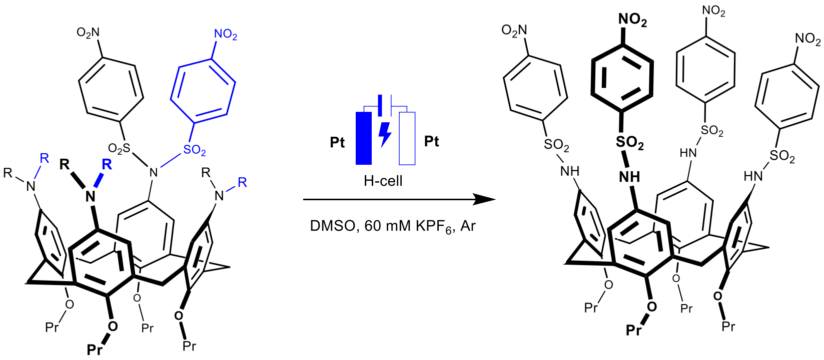

Figure 1: Electrochemical cleavage of octakis-nosylated calixarene.

alization employing triethylamine as a reductant to cleave C-halogen, N-C, O-S, O-C, C-C, and C-N bonds.

In this work, we describe the unexpected electrochemical cleavage of sulfonimides, providing a direct pathway to corresponding sulfonamides. For this purpose, 16 substances were synthesized and tested, reflecting the influence of different electron effects of -SO_2Ph-R substituents, and the impact of the number of nosyl units present in molecules. In the case of octakis-nosylated calixarenes, the electrochemical cleavage *via* direct potential-controlled electrolysis was compared with conventional organic synthetic procedures. After electrolysis, all prepared sulfonamides were isolated in excellent yields.

References

1. Hammerich O.; Organic Electrochemistry Revised and Expanded; 5th ed., CRC Press, Boca Raton **2016**.
2. Huang, B.; Guo, L.; Xia, W. *Green Chem.*, **2021**, *23*, 2095–2103.

Green approach for the preparation of biosourced ionic liquids and the study of their thermodynamic properties

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Supervisors: Prof. Sandrine Bouquillon, Ing. Magdalena Bendova, PhD.
Supervising Expert: Dr. Jean-Pierre Mbakidi

In the modern context of sustainable development as well as of the availability of raw materials of petrochemical origin and to the naturalness desired by consumers, the term “biosourced” appears ever increasingly.[1] The valorization of biopolymers such as lignin is one of the biggest challenge due to its complex structure, yet is nevertheless extensively studied from both the fundamental and industrial point of view.[2] While the three major entities of which lignin is composed are of great interest for chemical industry, finding ways of extracting these components proves challenging.[3] Indeed, for a few years, studies on the dissolution and the treatment of lignin have been developed to valorize this biopolymer. This presentation will address a green approach to the synthesis of ionic liquids qualified as biosourced (monocatenar or bolaform systems) from specific agro-resources, according to several principles of green chemistry. As these solvents could be used to solubilize lignocellulosic biomass and/or extract bioactive compounds (from plant sourcing), the physicochemical characteristics (density, viscosity and heat capacity) of pure ILs or mixtures of IL/water must be determined. Preliminary results concerning this last point will be presented.

References

1. Hulsbosch, J.; De Vos, D. E.; Binnemans, K.; Ameloot, R. *ACS Sustain. Chem. Eng.* **2016**, *4*, 2917–2931.
2. Sethupathy, S.; Morales, G. M; Gao, L.; Wang, H.; Yang, B.; Jiang, J.; Sun, J.; Zhu, D. *Bioresour. Technol.* **2022**, *347*, 126696–126712.
3. Xu, J.; Li, C.; Dai, L.; Xu, C.; Zhong, Y.; Yu, Y.; Si, Y. *Chem. Sus. Chem,* **2020**, *13*, 4284–4295.

Synthesis and cytotoxicity of fluorinated mannosamines

Student: Ing. Aleš Krčil
Supervisor: Mgr. Jindřich Karban Ph. D.

Fluorinated carbohydrates have been widely acknowledged as useful tools for studying the mechanisms of carbohydrate-processing enzymes and carbohydrate-binding proteins, as well as for inhibiting them.[1] The similarity in size between fluorine and hydroxyl has also led to research exploring the potential of fluorosugars to modify glycan chains by inhibiting carbohydrate-processing enzymes and/or altering the balance between carbohydrate metabolites. Although this research has identified several potent metabolic inhibitors, some fluorosugars have also been found to have cytotoxic effects, which also opens up the possibility of therapeutic applications.[2]

Non-fluorinated *N*-acetylmannosamine derivatives are cytotoxic, with their cytotoxicity depending on the substitution pattern of hydroxyl groups. Among the derivatives, 3,4,6-O-acylation resulted in the most cytotoxic acylated *N*-acetylmannosamines. Conversely, the 1,3,4-O-acylated N-acetylmannosamines exhibited significantly lower cytotoxicity, indicating that the position of O-acyl, and especially the presence of a free anomeric hydroxyl, play a crucial role in cytotoxicity.[3] Ensuing research showed that similar relationships between the cytotoxicity and O-acylation pattern also apply to *N*-acetylglucosamine and -galactosamine. In our previous study, we investigated the cytotoxicity of fluorinated acylated *N*-acetylgalactosamines and glucosamines. The results revealed that the introduction of fluorine increased cytotoxicity as long as the anomeric position remained unprotected.[4] On the basis of these findings, we have decided to expand our research to include fluorinated *N*-acetylmannosamines.

The aim of the project is to synthesise mono-, di- and trifluoro analogs of *N*-acetylmannosamines. The cytotoxicity of the final products towards selected cancer cells will be determined. The key intermediates are the corresponding multiply fluorinated mannosazide thioglycosides prepared from deoxyfluorinated 1,6-anhydro-2-azido-β-ᴅ-hexopyranose precursors by ring-opening reactions with phenyl trimethylsilyl sulfide.

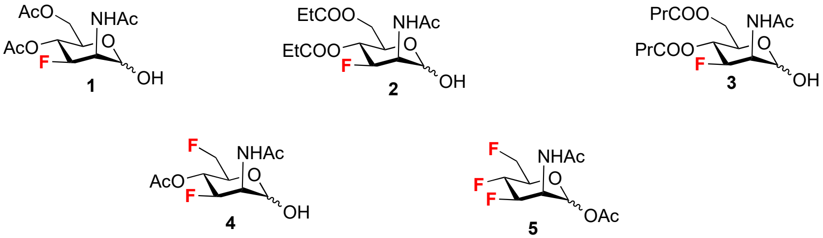

Figure 1: Structures of prepared fluorinated N-acetylmannosamine derivatives

References

1. Linclau, B.; Arda, A.; Reichardt, N. C.; Sollogoub, M.; Unione, L.; Vincent, S. P.; Jimenez-Barbero, J. *Chem. Soc. Rev.* **2020,** *49*, 3863–3888.
2. Goon, S.; Bertozzi, C. R. *J. Carbohydr. Chem.* **2002,** *21*, 943–977.
3. Almaraz, R. T.; Aich, U.; Khanna, H. S.; Tan, E.; Bhattacharya, R.; Shah, S.; Yarema, K. J. *Biotechnol. Bioeng.* **2012,** *109*, 992–1006.
4. Horník, Š.; Červenková Šťastná, L.; Cuřínová, P.; Sýkora, J.; Káňová, K.; Hrstka, R.; Císařová, I.; Dračínský, M.; Karban, J. *Beilstein J. Org. Chem.* **2016,** *12*, 750–759.

Chiral anion exchanger based on α-methylbenzylamine for enantioselective separation of racemic acids

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Supervising Expert: Doc. Ing. Zdeněk Slouka, Ph.D.

Chirality is a property of asymmetry that is responsible for the existence of enantiomers, molecules that are mirror images of one another. In a symmetrical environment, these molecules have the same chemical properties. However, the way in which they interact with other chiral substances, may be very different. Since human metabolism involves many stereoselective interactions, it is especially important to consider chirality during the development of new drugs, where the unwanted enantiomers may burden patients' organs or even be toxic. Preparation of enantiomerically pure drugs is, however, not always possible and the separation of racemic mixtures on larger than analytical scale has been a challenging task.

Among analytical methods, high performance liquid chromatography (HPLC) has been successfully used for the separation of many racemic chemicals. However, scale-up to preparative or industrial scale is typically not economically feasible. In this work, new enantioselective material based on α-methylbenzylamine as the chiral selector (recently utilized by our group in the preparation of chiral membranes[1]) covalently attached to Merrifield resin beads is proposed and discussed as a potentially cost-effective alternative to typically expensive stationary phase materials. It is shown that charged chiral methylbenzylamine works as an enantioselective anion exchanger potentially suitable for the separation of chiral acids, such as N–protected amino acid, or non-steroidal anti-inflammatory drugs (NSAID), such as ibuprofen. In a glass column chromatography experiment, racemic N–(tert–butoxycarbonyl) tryptophan was partially separated, reaching enantiomeric excess in eluates of around 10%.

References

1. Otmar, M.; Gaálová, J.; Žitka, J.; Brožová, L.; Cuřínová, P.; Kohout, M.; Hovorka, Š.; Bara, J. E.; Bruggen Van der, B.; Jirsák, J.; Izák, P. *Eur. Polym. J.* **2020**, *122*, 109381

Application of hydrodynamic cavitation in brewing

Student: Ing. Jiří Štěrba
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Supervising Expert: Ing. Miroslav Punčochář, DSc.

The positive role of hydrodynamic cavitation (HC) has been an object of study of the last two decades. HC phenomena involves the generation, growth, coalescence and subsequent implosive collapse of bubbles or cavities, occurring within a few microseconds and releasing large magnitudes of local pressure and temperature. Due to its very high oxidative capability in combination with mechanical shockwaves, HC processes can disrupt biological cells, destroy microorganisms, neutralize toxic chemicals or change molecule structures.

The aim of this work is to apply these advantages in the brewery industry. In the field of beer brewing, we would like to investigate several phenomenona, such as the isomerization of bitter hop acids, the reduction of gluten concentration or the cell-walls breakdown.

The first step of our work was the construction of the experimental setup formed by a special jet and pump control. A Venturi jet system with a special inclined tube was chosen as the HC technique due to energy savings and robust design. The process of cavitation was examined in more details. Hence, the Venturi tube was installed in a pilot scale brewery system.

Several experiments have been performed to confirm the positive effect of hydrodynamic cavitation on the isomerization of the hop bitter substances, and the influence in gluten removal due to the cavitation. Furthermore, several parts of the experimental brewery were improved. The regulation of individual parameters affecting the performance of HC was achieved due to equipment improvements.

Hydrodynamic cavitation is a very interesting phenomenon, which can see applications not only in the process of beer brewing, but also in the entire food industry. It is important to investigate this phenomenon, to find its mechanism and extend its applications.

Cultivation of *Limnospira maxima* and utilization of its fresh biomass in human nutrition

Student: Ing. Claudia Vásquez
Supervisor: Ing. Irena Brányiková, Ph.D.

The dried biomass of the cyanobacteria *L. maxima*, commonly known as "spirulina," is an available dietary supplement in powder or tablet form that has been linked to numerous positive effects on human health.[1] However, the process of drying and storing the biomass can result in oxidative reactions that damage important nutritional components and generate undesirable odors and flavors.[2] For this reason, the use of fresh biomass is a potential alternative that not only maintains the sensory qualities of the product, but also helps to preserve its nutritional value.[3]This work aims to enhance productivity, efficiency and sustainability of *L. maxima* cultivation as well as to determine the safe microbiological conditions for the nutritional use of fresh spirulina biomass. Various parameters such as light intensity, light spectral composition, temperature, pH, $CO_{2,}$ and culture media composition can be optimized. A series of experiments were performed to find the most suitable configuration to cultivate *L. maxima*, defined by cyanobacterium productivity and yield as well as other metabolites production such as phycocyanin (C-PC) and carotenoids. Procedures of photoautotrophic cultivation were mastered in volumes of 0.3 to 200 l, including methods of growth monitoring and related analytical procedures. The productivity of the culture at different illumination levels, cultivation temperatures and alternative sources of nitrogen showed that overall, *L. maxima* can grow in a wide range of conditions, being optimal at 30 °C , light intensity of $150\,\mu E \cdot m^{-2} \cdot s^{-1}$ and culture media with nitrate as N source, however, higher productivity was not necessarily related to higher production of valuable metabolites such as C-PC. In conclusion, this study has shown that *L. maxima* cells can grow in a wide range of conditions, however, the optimization of parameters can significantly enhance the productivity, efficiency, and sustainability of the cultivation, while also ensuring safe microbiological conditions for the nutritional use of fresh spirulina biomass.

References

1. Thevarajah, B.; Nishshanka, G. K. S. H.; Premaratne, M.; Nimarshana, P. H. V.; Nagarajan, D.; Chang, J. S.; Ariyadasa, T. U. Large-Scale Production of Spirulina-Based Proteins and c-Phycocyanin: A Biorefinery Approach. *Biochem. Eng. J.* **2022**, *185*, 108541.
2. Stramarkou, M.; Papadaki, S.; Kyriakopoulou, K.; Tzovenis, I.; Chronis, M.; Krokida, M. Comparative Analysis of Different Drying Techniques Based on the Qualitative Characteristics of Spirulina Platensis Biomass. *J. Aqua. Food Prod. Technol.* **2021**, *30* (5), 498–516.
3. Baranowski, J. D.; Dominguez, C. A.; Magarelli, P. C. Effects of Drying on Selected Qualities of Spirulina Platensis Protein. *J Agric. Food Chem.* **1984**, *32* (6), 1385–1387.

Use of photoautotrophic microorganisms in bioremediation of surface waters

Student: Mgr. Petra Mušálková
Supervisor: Ing. Irena Brányiková, Ph.D.

Eutrophication, an excess of nutrients (especially phosphorus) in water, has negative consequences, including massive harmful algal blooms, oxygen deficiency and toxin production, which can lead to the total collapse of water ecosystems. Although there are several procedures for dealing with eutrophication, they are expensive, have limited efficiency and/or involve the introduction of chemicals. Thus, we have been investigating phosphorus uptake by the cyanobacteria *Tolypothrix tenuis* as a potential agent for bioremediation. At the same time, we are developing a floating photobioreactor which would be placed on the eutrophic water body surface, and which will enable an exchange of water between its inner volume and the bulk water. In this bioreactor, intently cultivated harmless cyanobacteria will uptake the available nutrients, making them unavailable for the harmful species of algae. Afterwards, the obtained biomass will be harvested and used as a fertilizer in ecological agriculture.

Extensive experimental work has been executed to examine suitability of the proposed approach. Firstly, a study of *T. tenuis* growth and phosphorus uptake under the following conditions was conducted; *T. tenuis* was grown in standard BG media differing in initial biomass concentration (0.3, 0.8, 1.7 g/L), pre-inoculation conditions (0 mg/L of phosphorus for 0, 3, 6, 9 days), temperature (11, 15, 20, 25 °C), light intensity (60, 15, 250, 350 μE·m^{-2}·s^{-1}) and light regime (12:12h DLC). Secondly, we tested the suitability of floating bioreactor models for this bioremediation method. Throughout the experiments, phosphorus concentration in the media was measured spectrophotometrically; to confirm the amount of phosphorus uptake, the intracellular phosphorus concentration was analyzed by ICP-OES spectrophotometry. It was found out that *T. tenuis* was able to efficiently reduce the phosphorus concentration in the cultivation media, even to 0.02 mg/L which is considered a threshold for eutrophy. The reduction rate was proportional to the *T. tenuis* biomass concentration. The phosphorus-starved cultures had lower amounts of intracellular phosphorus, leading to a higher phosphorus uptake rate. Regard-ing temperature, lower temperatures slowed phosphorus uptake and biomass growth, but increased intracellular phosphorus concentration. Increased light intensity positively affected the phosphorus uptake and biomass growth, and finally day/night mode did not affect the phosphorus uptake rate. Overall, our results suggest that *T. tenuis* is a suitable organism for the water bioremediation.

Organic fluorine content and change during thermal treatment

Student: Ing. Matěj Hušek
Supervisor: doc. Ing. Michael Pohořelý, Ph.D.
Supervising Expert: Ing. Jaroslav Moško, Ph.D.

The variability of organic substances (pollutants) is constantly increasing as they are upgraded, substituted, or processed, making their detection more difficult and disproportionately expensive. Examples are per- and polyfluoroalkyl substances (PFAS), of which there are more than 9000 representatives,[1] and some have been confirmed to have a negative impact on human health.[2] Their use is widespread and variable (domestic and industrial), which affects their presence in sewage sludge[3]. We have previously described how pyrolysis affected the content of selected PFAS representatives.[4,5] However, we could not determine with certainty whether they were merely cleaved or mineralised. Therefore, we focused on the change in organic fluorine content (part of PFAS) and analysed its thermal behaviour in inert (sea sand) and heterogeneous (sewage sludge) material. The organic fluorine content decreased with pyrolysis temperature, but its concentration was a function of the pyrolysed material. The ability to measure organic fluorine includes PFAS, together with other organofluorine contaminants, such as pharmaceuticals or agrochemicals.[6] Setting aggregate limits, such as the total organic fluorine content, poses a challenge for future research, along with setting legislations of interest.

Acknowledgements

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References

1. EPA, PFAS Master List of PFAS Substances, **2023**.
2. Fenton, S. E.; Ducatman, A.; Boobis, A.; DeWitt, J. C; Lau, C.; Ng, C.; Smith, J. S.; Roberts, S. M. *Environ. Toxicol. Chem.*, **2021**, *40*, 606–630.
3. Semerád, J.; Hatasová, N.; Grasserová, A.; Černá, T.; Filipová, A.; Hanč, A.; Innemanová, P.; Pivokonský, M.; Cajthaml, T. *Chemosphere*, **2020**, *261*, 128018.
4. Hušek, M., Removal of PFASs from sewage sludge by pyrolysis. Prague: Institute of Chemical Process Fundamentals of the CAS, v. v. i., **2022**, 31-32. ISBN 978-80-86186-24-5. [Bažant Postgraduate Conference 2022. Prague (CZ), 13.–14.06.2022]
5. Hušek, M.; Moško, J.; Pohořelý, M. Sewage sludge treatment methods and P-recovery possibilities: Current state-of-the-art. *J. Environ. Manag.*, **2022**, *315*, 115090.
6. Han, J.; Kiss, L.; Mei, H.; Remete, A. M.; Ponikvar-Svet, M.; Sedgwick, D. M.; Roman, R.; Fustero, S.; Moriwaki, H.; Soloshonok, V. A. *Chem. Rev.*, **2021**, *121*, 4678–4742.

Hazardous components: A case study in textile waste management

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Textile waste, a problem that has been somewhat overlooked for many years, is now coming to the fore.[1] The textile value chain is long and complex, with over 8000 chemicals used in different manufacturing processes.[2] A wide variety of chemicals are used in the manufacture of textile products for the improvement of essential properties and performance of textiles. Chemicals used in textiles significantly improve their quality and appearance. However, the harmful effects of these chemicals can occur at various stages of textile production and processing, such as dyeing, printing and finishing, as well as during use by consumers and at the end-of-life stage.[3] There is a lack of safety information on the presence and use of all of these chemicals in consumer products.

In particular, dyes and pigments are usually toxic and ecotoxic because of the rather high content of heavy metals. Both wastewater and landfill leachate contain water-soluble heavy metal ions and compounds characterized by high persistence and bioaccumulation in the environment.[4] Per- and polyfluorinated alkyl substances (PFAS), which are widely used in the textile industry for their excellent oleophobic and hydrophobic properties, are another hazardous group with a high persistence and bioaccumulation capacity.[5]

The emission of chemicals throughout the life cycle of a textile product is one of the biggest sustainability issues, and the identification of potentially toxic compounds and their synergistic effects in end-of-life textiles is currently a major research gap. To fulfill this gap, leaching tests will be carried out as an advanced waste characterization method, simulating the geochemical behaviour of textile waste under real conditions. The results will be discussed with a view to obtaining specific chemical information on the hazardous chemicals that are used and emitted in practice.

References

1. Hole, G.; Hole, A. S. Improving Recycling of Textiles Based on Lessons from Policies for Other Recyclable Materials: A Minireview. *Sust. Prod. Cons.* **2020**, *23*, 42–51.
2. Kant, R. Textile Dyeing Industry an Environmental Hazard. *Nat. Sci.* **2012**, *04* (01), 22–26.
3. Shirvanimoghaddam, K.; Motamed, B.; Ramakrishna, S.; Naebe, M. Death by Waste: Fashion and Textile Circular Economy Case. *Sci. Total Environ.* **2020**, *718* (1), 137317.
4. Li, X.; Yang, Y.; Yang, X.; Li, J.; Li, S.; Tang, S. Determination of Polycyclic Aromatic Hydrocarbons in Textiles by Gas Chromatography-Mass Spectrometry. *AATCC J. Res.***2016**, *3* (6), 6–11.
5. Buckley, T.; Karanam, K.; Han, H.; Vo, H. N. P.; Shukla, P.; Firouzi, M.; Rudolph, V. Effect of Different Co-Foaming Agents on PFAS Removal from the Environment by Foam Fractionation. *Water Res.* **2023**, *230*, 119532.

Investigation of recycling possibilities of discarded photovoltaic solar panels

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The long-term growth of the installed capacity of solar photovoltaic energy production is now enhanced by both the current economic and energy crisis. The current global production of energy from solar photovoltaic panels is about 500 GW. In addition, it is expected to increase by up to 5 000 GW by the year 2050.[1] On the other hand, this source of energy is bonded with the production of waste in the form of old or discarded photovoltaic solar panels. In 2016, the mass of waste solar photovoltaic panels was estimated at 45 000 metric tonnes globally. By the year 2030 there is an expected mass of waste solar photovoltaic panels of 1.7–8 million metric tonnes and by 2050, 60–78 million metric tonnes.[2]

In the current market, the vast majority of photovoltaic panels sold are monocrystalline and polycrystalline types.[3] Both photovoltaic solar panels have the same structure, consisting of an upper glass layer, a second bonding layer of poly(ethylene-vinyl acetate) (abbr. EVA), a third (middle) layer formed by silicone cells and other metals, a fourth layer of EVA and a fifth (final) layer of polyvinyl fluoride.[4] According to mass composition, around 75% of a photovoltaic solar panel consists of glass, 10% of polymers, 10% of aluminium, 3% of silicon cells, 1% of copper, and significantly less than 1% is formed by silver (values are approximate).

Taking into account the economic value and mass content of individual fractions sparked interest as components of glass, metals, and silicon cells. The biggest current problem is the inefficient deliberation of individual layers and physical pre-treatment. This work aims to find an economically effective and industrially feasible method of how to recycle discarded photovoltaic solar panels. Performed experiments determined the exact composition of photovoltaic solar panels and the advantages and disadvantages of the treatment mentioned in the literature. Results will be used for a full-scale industrial unit design for solar photovoltaic panels recycling.

References

1. Venkatachary, S. K.; Samikannu, R.; Murugesan, S.; Dasari, N. R.; Subramaniyam, R. U. Economics and impact of recycling solar waste materials on the environment and health care. *Environ. Technol. Innov.* **2020**, *20*, 101130.
2. Ansanelli, G.; Fiorentino, G.; Tammaro, M.; Zucaro, A. A Life Cycle Assessment of a recovery process from End-of-Life Photovoltaic Panels. *Appl. Energy* **2021**, *290*, 116727.
3. Włodarczyk, R. Analysis of the Photovoltaic Waste-Recycling Process in Polish Conditions—A Short Review. *Sustainability* (*Switzerland*) **2022**, *14* (8), 4739.
4. Peplow, M. Solar Panels Face Recycling Challenge. *ACS Central Sci.* **2022**, *8* (3), 299–302.

Properties and use of high-temperature biochar

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Despite being a hot topic in environmental research, biochar and its properties have been mainly investigated from the perspectives of feedstock type and pyrolysis temperature. Few studies have explored the effect of particle size on biochar properties.[1] Even when the effect of particle size on crop efficiency is recognized, there is a lack of corresponding data and analysis.[2–7] Therefore, we thoroughly analyzed (proximate and ultimate analysis, SEM, XRD, Raman spectroscopy) four particle size fractions (< 0.5, 0.5–2, 2–5, > 5 mm) of high-temperature biochar from a gasification power plant, the sizes reflecting those of biochar actually used in agriculture. The < 0.5 mm fraction was significantly different in terms of carbon structure, and carbon and ash content; consequently, pH, electric conductivity and heavy metal content also differed greatly. The corresponding results for the other particle fractions were broadly similar to each other. Interestingly, for all fractions, the porosity and H/C ratio were independent of particle size, meaning that, regardless of size, the investigated biochar fractions are equally stable in soil. The 0.5–2 mm fraction was then selected to be used in different industrial or agricultural processes such as the anaerobic digestion of wastewater or livestock feeding. The effect of biochar on these processes is currently under investigation, providing only initial data so far.

References

1. He, P.; Liu, Y.; Shao, L.; Zhang, H.; Lü, F. Particle Size Dependence of the Physicochemical Properties of Biochar. *Chemosphere* **2018**, *212*, 385–392.
2. Prodana, M.; Silva, C.; Gravato, C.; Verheijen, F. G. A.; Keizer, J. J.; Soares, A. M. V. M.; Loureiro, S.; Bastos, A. C. Influence of Biochar Particle Size on Biota Responses. *Ecotoxicol. Environ. Saf.* **2019**, *174*, 120–128. .
3. de Jesus Duarte, S.; Glaser, B.; Pellegrino Cerri, C. Effect of Biochar Particle Size on Physical, Hydrological and Chemical Properties of Loamy and Sandy Tropical Soils. *Agronomy* **2019**, *9* (4), 165.

4. Werdin, J.; Conn, R.; Fletcher, T. D.; Rayner, J. P.; Williams, N. S. G.; Farrell, C. Biochar Particle Size and Amendment Rate Are More Important for Water Retention and Weight of Green Roof Substrates than Differences in Feedstock Type. *Ecol .Eng.* **2021**, *171*, 106391.
5. Alghamdi, A. G.; Alkhasha, A.; Ibrahim, H. M. Effect of Biochar Particle Size on Water Retention and Availability in a Sandy Loam Soil. *J. Saudi Chem. Soc,* **2020**, *24* (12), 1042–1050.
6. Głąb, T.; Palmowska, J.; Zaleski, T.; Gondek, K. Effect of Biochar Application on Soil Hydrological Properties and Physical Quality of Sandy Soil. *Geoderma* **2016**, *281*, 11–20.
7. Hussain, R.; Ghosh, K. K.; Ravi, K. Influence of Biochar Particle Size on the Hydraulic Conductivity of Two Different Compacted Engineered Soils. *Biomass Convers. Biorefin.* **2021**, *13* (2), 801–811.

Intercomparison of boundary layer and mixing layer height from models and ground-based measurements

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Introduction

The planetary boundary layer is the layer next to the Earth's surface, most affected by the vertical transfer of momentum, heat, and mass across the surface. It is also considered as a key parameter in air pollution modeling since most of the pollutants emitted from the surface become constrained within this layer due to lower vertical turbulent mixing above the planetary boundary layer.[1] The boundary layer characterized by vigorous vertical turbulences is known as the convective boundary layer (CBL) or mixing layer.[2] The turbulence can be caused by either wind or wind shears that generate mechanical turbulence (called forced convection), or by buoyant forces (called free convection) associated with large thermals. The boundary layer shows diurnal variation due to solar radiation, with the rising of the mixing layer during the daytime and shrinking at night.[3] There is a lack of studies on the reliability of boundary/mixing layer retrievals from the Reanalysis models, which are considered to capture the general pattern of the daily cycles relatively well, particularly for remote regions.

Methods

In the present study, we obtained the ERA5 (fifth-generation European Centre for Medium Weather Forecasting reanalysis model) [4] boundary layer and HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) [5] model based on GFS (Global Forecast System), GDAS (Global Data Assimilation System), and Reanalysis datasets on mixing layer height for the National Atmospheric Observatory Košetice (NAOK) (49°35′N, 15°05′E; 534 m a.s.l) for the year 2020.

For the ground-based measurements of the boundary layer and mixing layer height, the ceilometer model CL51 from Vaisala Inc. (Helsinki, Finland) was used. The ceilometer uses a LIDAR remote sensing technique to record the optical backscatter intensity in the infrared wavelength range (900 ± 10 nm) sent out in a vertical direction. Reflection and backscatter caused by clouds, precipitation, haze, fog, mist, and other obscurations are measured as the laser pulses traverse the sky. The backscatter profile is further used to detect the boundary layer and mixing layer height.

Results and Discussion

In this study, we found that the boundary layer height tends to be lower in ERA5 and timing for the daily peak also appears to differ as compared to ceilometer boundary layer data. In contrast, the ERA5 boundary layer observation was found to agree well with the mixing layer height obtained from the ceilometer. Whereas in comparison to HYSPLIT, GFS and GDAS, observations were found to agree well with ceilometer data while Reanalysis underestimated mixing layer height throughout the year. The seasonal changes in the boundary/mixing layer height were well captured by both models and the ceilometer.

This study also reveals that the models underestimated the mixing layer observations during the summer by 31%–45% and agreed relatively well during the winter season by a difference of 10%, although the surface temperature measured by models was found to follow the same trend as in-situ measurements. The additional variables such as global radiation, synoptic situation and stability of the atmosphere will also be studied to explain the difference.

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References

1. Hayden, K., et al. *Atmosph. Environ.* **1997**, *31*, 2089–2105.
2. Siebert, H., et al. *Boundary-Layer Meteorology* **2000**, *94*, 165–169. .
3. Mahrt, L. *Boundary-Layer Meteorology* **1999**, *90*, 375–396.
4. Hersbach, H., et al. *Quarterly J. Royal Meteo. Society* **2020**, *146*, 1999–2049.
5. Stein, A. F., et al.; *Bulletin Amer. Mete. Society* **2015**, *96*(12), 2059–2077.

Vertical gradients of atmospheric aerosols chemical composition

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Atmospheric aerosols differ in concentration and chemical composition with altitude above the Earth's surface. At higher altitudes, aerosol constitution is significantly influenced by long-range transport. The National Atmospheric Observatory Košetice with its 250 m high tower is a unique installation that enables the study of vertical gradient of atmospheric aerosols chemical composition over extended periods of time.

The aim of this work is to obtain data on the chemical composition of aerosols at two heights (4–5 metres above ground and at 230 metres on the atmospheric tower's measurement platform). The following analytical methods and sampling techniques will be used:

AMS (Aerosol Mass Spectrometry) – in combination with PMF (Positive Matrix Factorisation), this method deconvolves complex mass spectrum allowing us to distinguish individual chemical species or groups. Numerous field studies have demonstrated that aerosol mass concentrations and size distributions measured by AMS generally agree well with data acquired from other instruments.[1–4]

ACSM (Aerosol Chemical Speciation Monitor) – in contrast to AMS, the ACSM is simplified, compact-sized, lower-priced and does not provide particle size measurement. On the other hand, AMS features better mass resolution and detection limits.[5]

PILS-IC (Particle Into Liquid Sampler coupled with Ion Chromatography) – this technique is designed for the continuous monitoring of aerosol chemical composition. Particles are mixed with saturated vapour generated from ultrapure water, forming droplets that are then collected.[6,7] Liquid-phase samples are analysed with IC or can also be stored frozen and analysed with other methods of choice. PILS-IC provides near real-time measurements for long-term operation. Additionally, accessory denuders will be applied. These denuders cut off any influence of species present in ambient air in the gas phase.[8]

Filtering – the oldest method for aerosol chemical composition analysis still plays an irreplaceable role. Various materials can be used (fibrous – e. g. glass, polymer; and porous – e.g. polycarbonate, cellulose), each of them having advantages and disadvantages. The most commonly used material is quartz fibre; universal but suffers from high levels of hygroscopicity.

Results obtained using the above mentioned analytical methods and sampling techniques will be evaluated with regard to meteorological parameters, mainly atmospheric conditions such as boundary layer height and gradient of wind speed and direction. The contribution of long-range transport on concentration of individual species will be also evaluated. Online methods of aerosol mass spectrometry (AMS/ACSM) as well as semi-online (PILS) and offline (filters) will be used and compared. Chemical composition will be also evaluated with regard to daily and seasonal cycles.

References

1. Allan, J. D. et al. *J. Aerosol Sci.* **2004**, *35*, 909–922.
2. Bae, M. S. et al. *Aerosol Sci. Technol.***2007**, *41*, 329–341.
3. Takegawa, N. et al. *Aerosol Sci. Technol.***2005**, *39*, 760 – 770.
4. Salcedo, D. et al. *Atmos. Chem. Phys.***2006**, *6*, 925–946.
5. Fröhlich, R. et al. *Atmos. Meas. Tech* **2013**, *6*, 3225–3241.
6. Khlystov, A. et al. *Atmos. Environ.***1995**, *29*, 2229–2234.
7. Simon, P. K. and Dasgupta, P. K. *Anal. Chem.***1995**, *67*, 71–78.
8. Orsini, D. A. *Atmos. Environ.***2003**, *37*, 1243–1259.

The effect of meteorology and aerosol size distribution on light scattering properties at a rural background site in Central Europe

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Atmospheric aerosols have a significant impact on the Earth's radiative forcing.[1] They affect the Earth's climate system directly by scattering or absorbing incoming solar and outgoing infrared radiation, and indirectly by altering cloud properties and their lifetime.[2] The reasons for the large uncertainty of aerosols in climate modeling are not yet fully understood. Although there are studies that address the effects of aerosols on local climate,[3–5] there are few long-term series measured at rural background sites.

The aim of this study is to characterize the light scattering properties of aerosols at the rural background site National Atmospheric Observatory Košetice (NAOK; 49°34′20.787″N, 15°4′48.155″E) in Central Europe, namely the coefficients of total light scattering (σ_{sp}) and backscattering (σ_{bsp}), the Ångström exponent (SAE), the backscattering ratio (b), and the asymmetry factor (g), with special attention to the influence of meteorology and aerosol size distribution on these properties. We measured σ_{sp} and σ_{bsp} at three wavelengths (450, 550, and 700 nm) using the Integrating Nephelometer TSI 3563 (PM_{10} inlet). The measurements were performed from August 16, 2012 to December 31, 2019.

The results show an interannual downward trend in σ_{sp} and σ_{bsp} associated with a shift toward larger particles and an enhanced aerosol cooling effect during the observed period. Increased SAE values in summer indicate increased SOA formation, while the decrease in b in winter indicates increased concentrations of carbonaceous aerosols. The σ_{sp} and σ_{bsp} values were higher during fog events, medians $76.71\,\mathrm{Mm}^{-1}$ and $8.57\,\mathrm{Mm}^{-1}$ compared to no fog events, with $34.82\,\mathrm{Mm}^{-1}$ and $5.21\,\mathrm{Mm}^{-1}$ at 550 nm, respectively, due to increased particle size during fog events. The value of g showed a decreasing scattering potential of particles during fog events, possibly due to multiple scattering of light by the particles. Higher values of σ_{sp} and σ_{bsp}

were observed during overcast and fine days compared to cloudy or partly cloudy days ($p < 0.05$). The optical properties of aerosols correlated most strongly with the presence of particles between 200 and 800 nm, close to the wavelength of visible light.

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References

1. Bäumer, D.; Vogel, B.; Versick, S.; Rinke, R.; Möhler, O.; Schnaiter, M. *Atmos. Environ.* **2008**, 42, 989–998.
2. IPCC. Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change., **2013**.
3. Luoma, K.; Virkkula, A.; Aalto, P.; Petäjä, T.; Kulmala, M. *Atmos. Chem. Phys.* **2019**, 19, 11363–11382.
4. Delene, D. J.; Ogren, J. A. *J. Atmos. Sci.* **2002**, 59, 1135–1150.
5. Pandolfi, M. et al. *Atmos. Chem. Phys.* **2018**, 18, 7877–7911.

N-alkylation of a lysergic acid derivative under PTC conditions in a continuous arrangement using sonication

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Supervising Expert: Ing. Petr Stavárek, Ph.D.

This contribution focuses on the application of sonication to the synthesis of a methyl ester of the 1-methyl-10α-methoxydihydrolysergic acid (MeLUME). The N-alkylation reaction takes place under phase transfer catalyzed conditions.[1,2] The alkylation was performed in a continuous regime.[3] This reaction in a batch reactor is included in the industry's production of the drug Nicergoline, prescribed to patients with Alzheimer's disease and dementia.[4] The reaction proceeds in two immiscible phases, and to increase the space-time yield, the effect of sonication was examined. Sonication led to a more intensive renewal of the interfacial area and hence intensification of a mass transfer of reaction components through the interface. First experiments with sonication were in an apparatus with a FlowPlate microreactor (LONZA), where the sonication was applied to the outlet capillary, that represented asignificant part of the reaction volume. The positive effect of sonication on the course of the reaction was observed. Therefore, the new reactor from static micromixers on a modular microreactor system was assembled. This reactor could be completely immersed into the sonication bath. However, the results achieved using this apparatus did not reach the values obtained from the previous measurements with the LONZA reactor. Based on the obtained knowledge, a new type of reactor consisting of a fluoropolymer (FEP) capillary was assembled. The results obtained after optimization of the reaction process in this reactor were comparable to those achieved in the LONZA reactor. The use of sonication for the N-alkylation reaction allowed for doubling of the amount of product synthetized while maintaining high conversion and selectivity.

References

1. Cvak, L.; Stuchlik, J.; Cerny, A.; Krepelka, J.; Spacil, J. Dihydrolysergol's 1-alkylated derivatives preparation method. CS234498B1, 1984.

2. Cvak, L.; Stuchlik, J.; Roder, L.; Markovic, L.; Krajicek, A.; Spacil, J. Method of dihydrolysergol's N1 alkylated derivatives preparation. CS247570B1, 1988.
3. Nieves-Remacha, M. J.; Torres, M.; Ruiz-Abad, M.; Rincon, J. A.; Cumming, G. R.; Garcia-Losada, P., Scale-up of N-alkylation reaction using phase-transfer catalysis with integrated separation in flow. *React. Chem. Eng.* **2019,** *4* (2), 334–345.
4. Winblad, B.; Fioravanti, M.; Dolezal, T.; Logina, I.; Milanov, I. G.; Popescub, D. C.; Solomon, A., Therapeutic use of Nicergoline. *Clin. Drug Invest.* **2008,** *28* (9), 533–552.

Separation of exosomes from polydisperse suspension in microfluidic devices

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Exosomes are membrane vesicles with sizes ranging from 30 to 200 nm secreted by almost all mammalian cells. They play a pivotal role in cell-to-cell communication and in transferring various biomolecules such as proteins, microRNAs, and DNAs. Research on exosomes is mainly focused on exploiting their potential as biomarkers for disease diagnosis and their possible use in therapeutic applications such as drug delivery and tissue regeneration. As a result, their involvement in various physiological and pathological processes, including immune response and cancer progression, has been intensively studied in recent years.[1]

The extraction of exosomes from biological materials results in polydisperse suspensions containing the desired nanoparticles as well as various cells and debris. For biomedical purposes, it is necessary to carry out their separation. However, these vesicles are susceptible to mechanical damage, and current conventional separation methods, such as ultracentrifugation and filtration, risk sample degradation complicating the practical use of exosomes. Therefore, research in this area has focused on non-destructive methods as is, for example, the separation method based on microfluidic viscoelastic flow. In microfluidic devices, viscoelastic fluids are used to create controlled flow patterns that can selectively separate particles of different sizes by experiencing both viscous drag and elastic lift forces. The balance between these forces can cause specific particle migration. By carefully designing the flow conditions (flow rate, channel geometry) and fluid properties (viscosity), it is possible to exploit this migration behavior to separate exosomes from larger contaminants. Smaller particles like exosomes will experience less elastic lift and migrate closer to the channel walls, while larger particles are pushed toward the channel center.[2] These microfluidic viscoelastic flow-based separation methods offer several advantages, including low sample volume requirements, high-throughput processing, minimal sample dilution, and reduced risk of sample degradation. However, challenges remain in optimizing fluid properties and device designs for specific applications and ensuring the scalability and reproducibility of these techniques.

The research on exosome separation from polydisperse suspensions, where particle diameters vary in the range of 100-1000 nm, was carried out experimentally and with the help of numerical simulations. The work included fine-tuning the experimental methodology, writing an in-house code for exosome tracking based on a one-way approach, and performing a parametric study to investigate the separation potential of the microdevice as a function of channel geometry, flow rate, and viscosity. Preliminary results show that viscoelastic microfluidics can be used as an alternative to conventional exosome separation techniques.

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References

1. Janouskova, O.; Herma, R.; Semeradtova, A.; Poustka, D.; Liegertova, M.; Malinska, H. A.; Maly, J. Conventional and Nonconventional Sources of Exosomes–Isolation Methods and Influence on Their Downstream Biomedical Application. *Front. Mol. Biosci.* **2022**, *9*, 846650.
2. Liu, C.; Guo, J.; Tian, F.; Yang, N.; Yan, F.; Ding, Y.; Wei, J.; Hu, G.; Nie, G.; Sun, J. Field-Free Isolation of Exosomes from Extracellular Vesicles by Microfluidic Viscoelastic Flows. *ACS Nano* **2017**, *11* (7), 6968–6976.

Liquid mixing time and gas holdup in a bubble column bioreactor

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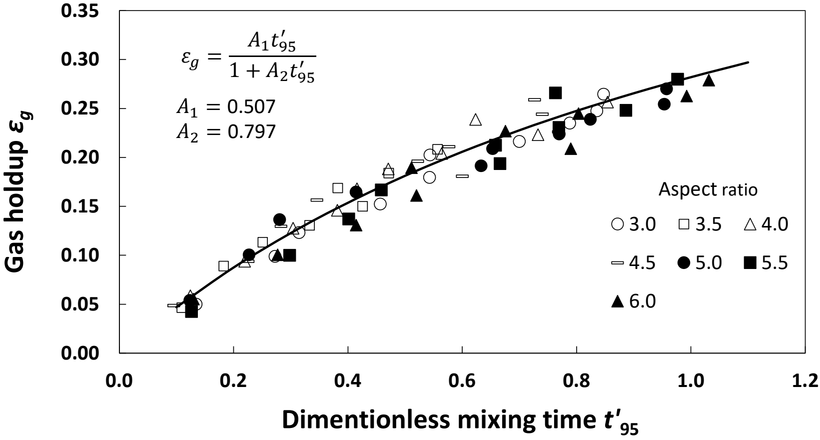
Supervising Expert: Sandra Cristina Kordač Petronilho Orvalho, Ph.D.

Bioreactors are widely used across many sectors of industry, especially in pharmacy and food production. Bubble columns are one of the bioreactor types suitable for cultivation of organisms sensitive to high shear forces, which often require careful supply of oxygen and other important nutrients. Therefore, controlled aeration and homogenization need to be established, especially in the case of tall bubble columns with high aspect ratios (liquid height to column width).[1] The aim of the research is the experimental study of homogenisation and aeration in a bubble column in dependence on operational conditions and aspect ratio.

Experiments were carried out in a bubble column with an inner diameter of 0.19 m, gas flow rate in the range 2–20 m^3/h and aspect ratios ranging in 3.0–6.0. Aeration was quantified by gas holdup measured from the change of dispersion height. Homogenisation was quantified by mixing time t_{95} measured via the colorimetric method based on tracer experiments. Acid and alkaline solutions were used



as tracers and concentration changes were visualized by a pH indicator. Colour changes were recorded by camera and evaluated via image processing.[2]

Obtained results provide a significant influence of aspect ratio on both gas holdup and t_{95}. Based on data analysis, a correlation between t_{95} and gas holdup was developed considering an influence of operation conditions and aspect ratio.

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References

1. Garcia-Ochoa, F.; Gomez, E. Bioreactor scale-up and oxygen transfer rate in microbial processes: an overview. *Biotechnol. Adv.* **2009**, *27* (2), 153–176.
2. Rosseburg, A.; Fitschen, J.; Wutz, J.; Wucherpfennig, T.; Schlüter, M. Hydrodynamic inhomogeneities in large scale stirred tanks – Influence on mixing time. *Chem. Eng. Sci.* **2018**, *188*, 208–220.

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

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

One of the possible techniques for non-invasive measurement of wall shear stress is the electrodiffusion method developed by Reiss and Hanratty.[2,3] The basic principle of the electrodiffusion method is to measure the limiting electric current flowing through the electrode flush-mounted with the wall. On the basis of the value of the electric current it is subsequently possible to describe hydrodynamics near the wall. Nevertheless, in order to obtain the studied hydrodynamic quantities from the electric current signal, appropriate relationships are needed, which can be found either by performing a calibration or by using a theory that analytically describes the investigated problem. The theoretical approach is based on the calculation of the mass transfer coefficient from measured electric current. However, to simultaneously determine the magnitude and direction of the wall shear stress, two independent electrical signals are desired, and thus the need arises for the use of a two-segment measuring probe.

This contribution deals with a new theory[4] describing 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. At the same time, 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 for different measuring probe geometries, 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.

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References

1. Havlica, J.; Kramolis, D.; Huchet, F. *Int. J. Heat Mass Transf.* **2021**,165, 120610.
2. Reiss, L. P.; Hanratty, T. J. *AIChE J.* **1962**, 8, 245-247.
3. Reiss, L. P.; Hanratty, T. J. *AIChE J.* **1963**, 9, 154-160.
4. Harrandt, V; Kramolis, D.; Huchet, F.; Tihon J.; Havlica, J. *Int. J. Heat Mass Transf.* **2023**, article accepted for publication.