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Optimization of Continuous Synthesis of Trazodone

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The project is based on a previous study of the continualization of the N-alkylation reaction under phase transfer catalysis conditions. The aim of the project was to validate the obtained procedures and knowledge by application to the synthesis of the drug Trazodone. This study explores the feasibility of synthesizing Trazodone in continuous mode using a tubular reactor and investigates the impact of ultrasound on phase-transfer catalyzed (PTC) N-alkylation[1,2]. One of the suitable approaches for a continuous system was solid-liquid arrangement described by Jaśkowska et. al [3], while synthesis is carried out in two steps with ultrasound assistance. The hypothesis for the reaction intensification with solid-liquid arrangement is that sonication accelerates transport at the solid-liquid interface and thus intensifies the reaction[4,5].

A continuous flow system was developed to perform the initial step of the reaction, with process conditions optimized to deliver yields comparable to those of the batch process (44–66i%). Efforts to directly adapt the solid-liquid (S-L) batch synthesis into a continuous setup were not successful. As an alternative, a novel liquid-liquid (L-L) strategy was established for synthesizing 2-(3-chloropropyl)-1,2,4-triazolo[4,3-a]pyridin-3(2H)-one (TAP). In this L-L system, the aqueous phase contained TAP, potassium carbonate, and tetrabutylammonium bromide, while the organic phase consisted of 1-bromo-3-chloropropane dissolved in ethyl acetate.

Several key parameters such as temperature, reagent excess, and residence time were systematically studied to evaluate their effects on TAP transport and product yield. On the basis of the experimental data, the apparent activation energy and reaction rate constant were determined. The reaction followed pseudo-first-order kinetics. The application of ultrasound irradiation led to a significant enhancement, boosting the yield by approximately 20i% at a residence time of 60 minutes.

The knowledge gained during the study of the first step of the synthesis was subsequently applied to the second step, where the Trazodone itself is produced. The solvents remained the same as in the previous case, as did the phase transfer catalyst. The first important step was to develop an HPLC method and to test the feasibility of the reaction in a packed bed and then in a continuous arrangement. The first results obtained show that better yields are achieved using the continuous apparatus than in the batch arrangement.

Acknowledgements

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Vertical Distribution and Precipitation Scavenging of Aerosols in a Rural Atmosphere: Insights from Winter 2019 to Spring 2020

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Vertical profiling of aerosols is essential to understand their atmospheric behavior, transformation, and health/climate impacts[1]. Black Carbon (BC), Organic Carbon (OC), and other aerosol components exhibit significant variability in concentration with height, especially under changing meteorological conditions[2]. Yet, limited studies have examined the vertical profiles of aerosols at rural background sites for longer periods of time.

This study investigates aerosol concentration profiles at two vertical levels—4 m and 230 m—in Central Europe, covering winter 2019 to spring 2020. The research was conducted at the National Atmospheric Observatory Košetice (NAOK), a regional background site with a 250-meter meteorological tower enabling the simultaneous measurement at 4 m and 230 m. The key aerosol components analyzed include equivalent black carbon (eBC), organic carbon (OC), elemental carbon (EC), and secondary inorganic aerosols (SO_4^{2-}, NO_3^-, NH_4^+).

The findings reveal that while the boundary layer is generally well mixed, most aerosol components show higher concentrations near the ground, with vertical ratios (230 m/4 m) typically between 0.5 and 0.8 (Figure 1). However, episodes of elevated concentrations at 230 m highlight the role of atmospheric dynamics and vertical transport mechanisms. Strong vertical gradients emerged during the boundary layer below 230 m, revealing surface-level pollutant accumulation. Fog events led to chemical processing and enhanced chloride/nitrate levels. Windy conditions caused dilution at both levels, with occasional aerosol enhancement aloft, indicating regional transport. Rain events demonstrated clear species-dependent scavenging, with SO_4 and NH_4 effectively removed, while eBC often showed a negative scavenging ratio, confirming its scavenging resistance.

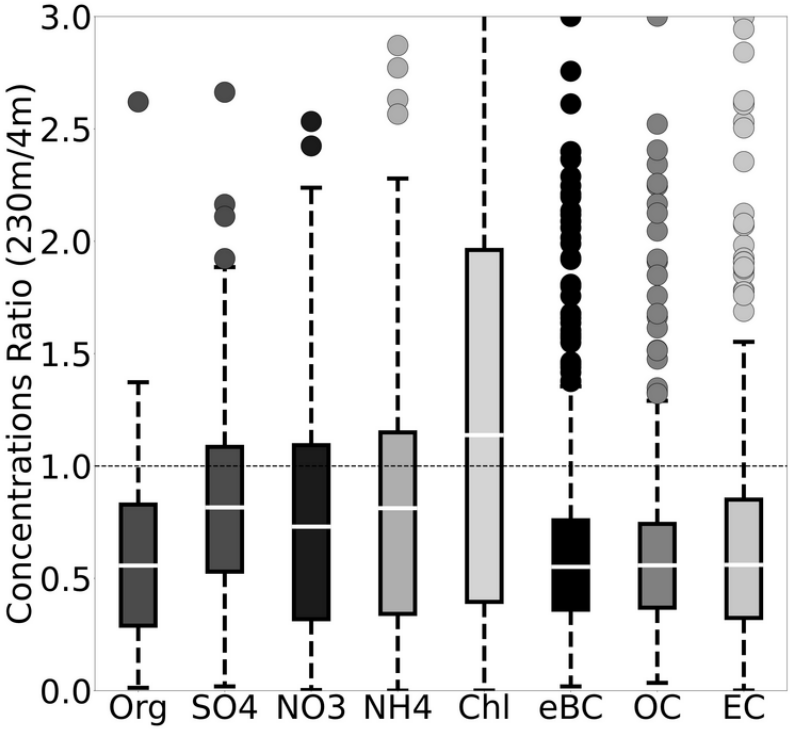

Figure 1: Boxplot of vertical concentration ratios (230 m / 4 m) for different aerosol species.

Acknowledgements

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Fluorinated Methyl B-lactosides and Their Multivalent Presentation

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Human galectins (*h*gals) are carbohydrate-binding proteins that have the ability to regulate immune responses and processes related to neoplastic transformation by recognizing galactoside-containing glycans.[1] Consequently, there has been a growing interest in developing selective galectin inhibitors. However, due to high structural similarity of galectins and overlapping glycan specificity, the design of selective inhibitors remains challenging. A deeper understanding of the distinctions between individual *h*gals could aid in the development of galectin inhibitors. Deoxyfluorinated carbohydrates, in which at least one hydroxyl group is replaced by fluorine, closely mimic natural ligands and allow for detailed probing of carbohydrate–protein interactions.[2] Systematic deoxyfluorination of a given galectin ligand enables the evaluation of the importance of each individual hydroxyl group of this ligand for the interaction with galectins. This can reveal subtle differences between various galectins, which is crucial for the development of selective inhibitors. Interactions between galectins and fluorinated ligands can be studied using ^{19}F NMR spectroscopy, leading to a more effective description of their molecular mechanism.[3]

This work is focused on a full series of mono-deoxyfluorinated methyl β-lactosides, synthesized via glycosylation of methyl glucoside with appropriately protected galactose donors, followed by deprotection. These derivatives are designed for affinity testing with selected human galectins using ELISA. Additionally, a strategy for multivalent ligand presentation is introduced: corresponding β-lactosyl azides were prepared for conjugation onto dendritic scaffolds via click chemistry. These multivalent constructs are useful for studying cluster effects and enhancing binding in lectin–glycan interactions.[4]

The presented compounds provide a structurally consistent set of fluorinated ligands suitable for comparative galectin binding studies

and represent a starting point for future glycomimetic optimization and scaffold-based ligand display.

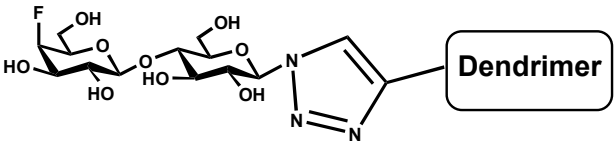

Figure 1: Example of β-lactosyl ligand conjugated to a dendrimer via triazole linker

Acknowledgements

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Quantifying Separation Quality of LARCODEMS: From Reference Plastic Mixtures to WEEE Streams

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The LARCODEMS device (an acronym derived from LARge COal DEnsity Medium Separator) is a type of density separator that operates on the basis of the sink-float process. If the density of the liquid lies between that of the two particle kinds, the lighter particles rise to the surface, whereas the heavier ones settle at the bottom. LARCODEMS generates a vortex that accelerates the separation process and also operates in a continuous mode.

In addition to the primary use in coal separation, various other applications have been explored, including the separation of plastic waste[1]. The importance of this application is becoming increasingly evident. Physical separation has been identified as a suitable preliminary step in plastic recycling, with several authors suggesting that enhancing the efficiency of physical separation may lead to higher yields of chemical methods used in downstream treatment[2,3]. Furthermore, this step has been identified as one of the key limitations[4].

This study investigates the separation efficiency of the device using a reference mixture of plastics. The separation of a mixture of eleven plastics with known densities was performed using various separation media (aqueous solutions of inorganic salts). The densities of separation media were measured. The particles were passed through the device and subsequently trapped on screens. Thereafter, they were thoroughly washed with water. Following the drying process, both fractions were manually sorted, and the individual plastics were weighed. The density of the separation medium was used to distinguish between the light and heavy fractions. The separation efficiency was calculated based on the weights of the individual plastics. It was determined that the LARCODEMS device can achieve high efficiency, even when the density difference between the separated particles is minor.

The separation process was additionally tested on a real sample of plastics obtained from the shredding of WEEE. The aim was to separate plastics from metals, with the separation quality assessed based on the metal content in both light and heavy fractions. It was found that the heavy fraction was significantly enriched with metals.

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Effect of Liquid Composition on Hydrodynamics in Bubble Column with Different Gas Distributors

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Aeration in bubble columns and other bioreactors is essential for proper cultivation and production. Design of efficient aeration needs determination of the volumetric mass transfer coefficient $k_L a$, which requires solid understanding of the system's hydrodynamics[1]. Hydrodynamics are studied through parameters like gas holdup ε_G, mixing time t_{95} and axial dispersion coefficient D_a. However, measurements of t_{95} and D_a are based on tracing methods that can alter the properties of the liquid phase leading to changes in hydrodynamics[2]. This work investigates how tracer addition typical for t_{95} and D_a determination affects system hydrodynamics and ε_G across different operating conditions. A better understanding of these changes will further help to reliably describe and control the hydrodynamics and mass transfer in bubble columns.

Experiments were conducted in a bubble column with inner diameter 0.19 m, using distilled water as a reference liquid and distilled water with various tracer compounds (KCl, NaOH, HCl and bromothymol blue BB). Batches were prepared to match previous experiments for D_a (KCl) and t_{95} (HCl + NaOH + BB). The concentrations of KCl were in the range from 0.040 to 0.400 g/l, and 0.001 to 0.040 g/l for HCl and NaOH. The concentration of bromothymol blue was always 0.006 g/l. The tested superficial gas velocities were in range from 0.02 to 0.20 m/s and tested aspect ratios (liquid height to column diameter) in the range from 3.0 to 6.0. Two different perforated plates were used as gas distributors. Both distributors had active area of 0.2%, but different orifice size: plate A had orifice diameter 1.6 mm producing pure heterogeneous regime and plate B had orifice diameter 0.5 mm producing three flow regimes (homogeneous, transition, and heterogeneous) depending on gas flow rate.

The results show different behaviour between plate A and B. For plate A, the change of ε_G depends on tracer used. Compared to distilled water, the addition of KCl increased the ε_G by 11% while the addition of HCl, NaOH and BB increased the ε_G by 34%. For plate B, the change of ε_G depended on current flow rate and flow regime. For the KCl the difference in ε_G compared to distilled water was up to 65% in homogeneous regime, up to 112% in transition regime and decreases to 41% in heterogeneous regime. For the batch containing HCl, NaOH and BB the difference in ε_G was even more significant up to 73% in the homogeneous regime, up to 155% in the transition regime and again the decrease to 47% in the heterogeneous regime. Based on the results, distilled water has considerably different hydrodynamic behaviour than batches containing tracers, which change the gas holdup ε_G significantly. Nonetheless, correlation of $k_L a$ and ε_G with D_a and t_{95} can be possible, but the tracers and tracer induced changes must be taken into consideration and proper correction must be made.

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Effect of Particle Size on Monodisperse Granular Mixing Process by Using Discrete Element Method

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Efficient mixing of granular materials is a fundamental operation in industries such as pharmaceuticals, food processing, and materials manufacturing. While particle size is known to significantly influence mixing dynamics, the underlying mechanisms governing this relationship remain incompletely understood[1]. This study systematically investigates how particle diameter affects mixing efficiency in a vertical cylindrical mixer using the Discrete Element Method (DEM).

Our simulations employed a Hertz-Mindlin contact model for spherical particles with diameters ranging from 0.25 mm to 4 mm. The mixer was equipped with dual flat blades operating at either 15 rpm or 150 rpm. Three distinct initial particle arrangements were tested: tangential (particles separated by a vertical plane), radial (particles separated by a cylindrical surface, with one type inside and the other outside), and axial (particles are separated by a horizontal layer). Two friction coefficients (0.1 and 0.5) were studied to assess the combined effect of particle friction and size. To isolate size effects, the total mass of particles was maintained constant across all simulations by adjusting particle numbers accordingly.

Quantitative analysis of mixing indices revealed that mixing efficiency consistently increased with particle diameter. This enhancement results from the higher inertia-to-dissipation ratio of larger particles, allowing for sustained momentum through fewer collisions. The tangential initial configuration consistently achieved faster homogenization, resulting in a shorter mixing time compared to axial and radial configurations under all tested conditions. A significant behavioral transition was identified between 1 mm and 2 mm particle

diameters. Particles smaller than this threshold exhibited primarily dissipation-dominated behavior with limited mixing, while larger particles displayed inertia-dominated dynamics with more efficient mixing. This transition was particularly pronounced at lower rotational speeds (15 rpm). These findings provide practical guidelines for mixing applications: when possible, selecting particles above the identified size threshold, utilizing tangential loading configurations, and understanding the interplay between particle size and operational parameters can significantly enhance mixing efficiency in granular processes.

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Theoretical Basis for Directional-sensitive Measurements Using Rounded Electrodiffusion Probes

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A highly valuable source of information for addressing various engineering, scientific, or biomedical questions is the research in the field of near-wall transport phenomena. In this context, we define two main areas of interest, namely the bulk of the fluid and the solid surface wall. The mediator between these areas is the so-called boundary layer, where the most abrupt changes occur in the entire system under study. One of the key quantities within the boundary layer is the wall shear stress, which represents the rate of change of fluid velocity at the wall and is directly related to the momentum transfer between the fluid core and the solid surface. With knowledge of this quantity, the possibility of a hydrodynamic description arises, and hence our interest in determining wall shear stress should be prominent, whether for the environmental, energetic, or chemical sectors[1].

Many measurement techniques have been developed to obtain the wall shear stress, whether through traditional mechanical methods, thermal methods, or optical methods. However, all of these groups suffer from certain shortcomings, and the electrodiffusion (ED) method stands out as the standout technique. The basic idea of the ED method is to measure the limiting diffusion electric current that flows through the circuit due to the ongoing redox reactions on the surfaces of the electrodes embedded in the wall surface where the shear stress is to be measured[2]. The shape of the measuring electrodes is a crucial factor during the measurement process, and the complexity of the geometric shape typically reflects the complexity of the problem being studied.

This work aims to establish a new theoretical foundation for ED probes that adopt a rounded shape. Attention is paid to probes that are formed by two semicircular segments. Although these probes have been applied in the past, a new theory[3] has been derived that enables

their application to directional sensitivity measurements. Furthermore, a new type of probes in the form of circular segments is proposed, which are obtained as a generalization of the twin semicircular shape when the variable position of the partition line is considered. The primary outcome of this work is the derivation of explicit analytical relations that describe the mass transfer to the probe sub-segments, depending on the geometry and direction of the flowing fluid. The correctness of the formulas is confirmed by numerical solution of the convection-diffusion equation. The study is further enriched by a sensitivity analysis, which aims to determine the optimal geometries for diagnosing the experimental measurements. Thus, the newly proposed theoretical procedures provide unprecedented opportunities for experimental fluid mechanics studies.

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Effect of Young's Modulus on Mixing Dynamics and Heat Transport in Granular Materials

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Heat transfer in granular materials plays a vital role in many industrial processes such as chemical reactions in stirred reactors or drying operations. In recent years, significant progress has been made in understanding thermal transport in these systems through both computational modelling and experimental studies. The Discrete Element Method (DEM) presents as a powerful tool, offering a detailed alternative to physical measurements[1].

DEM is a numerical method that simulates the movement of individual particles of a material by solving force and thermal energy balances of these particles. In systems where gas conduction and convection are negligible, and radiation is minimal due to lower temperatures, we consider only conduction in the solid phase as the primary heat transfer mechanism[2].

The primary objective of this study is to investigate Young's modulus and its effect on mixing dynamics, as well as on the transfer of heat in granular materials within a vertical cylindrical mixer equipped with heating jackets and with two opposing flat blades using DEM simulations. We investigated Young's modulus ranging from 5×106 to 5×1010 Pa and stirrer rotational frequencies from 0 to 240 rpm. This study provides a detailed evaluation of parameters such as contact time and contact area, which are strongly influenced by material stiffness, specifically Young's modulus, and stirrer rotational speed. These parameters have a direct impact on heat transfer. The results show that choosing unrealistically low modulus values to reduce computational cost by allowing larger time steps exaggerates particle contact and overestimates heat flux. In contrast, realistic Young's modulus values shorten collision duration and reduce the effective conductive contact area, revealing a more physically accurate rate of heat transfer. This work demonstrates that while artificially lowering the Young's

modulus may be sufficient for purely dynamic studies, accurate thermal transport modeling requires careful selection of stiffness.

Acknowledgements

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

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Visible-light Degradation of Tetracycline Using Porous g-C_3N_4 Coatings

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Graphitic carbon nitride (g-C_3N_4) has emerged as a promising metal-free photocatalyst, thanks to its chemical stability, suitable band gap (2.7 eV), and ability to utilize visible light. In this study, we focus on the development of g-C_3N_4 thin films for pollutant degradation in a slit-geometry photo-microreactor, with particular attention to the effect of film porosity induced by a camphor-based porogen.

The g-C_3N_4 photocatalyst was synthesized through thermal condensation of a melamine cyanurate, a supramolecular complex, at 550 °C under a nitrogen atmosphere[1]. The resulting powder was ball-milled and used to prepare coatings containing varying amounts of camphor (0–48w/w) as a porogenic agent. A plasma treatment was applied to enhance surface hydrophilicity. The morphology and composition of coatings were characterized using XPS, ATR-FTIR, SEM, profilometry, and nitrogen sorption at 77 K. Tetracycline (TET) was used as a model pollutant to evaluate photocatalytic performance, and degradation products were analyzed by HPLC-MS.

Spectroscopic data confirmed that camphor did not alter the chemical structure of the g-C_3N_4 matrix. Among the tested samples, the coating containing 32% camphor (D32K) demonstrated the best combination of surface uniformity and mechanical stability. Surface area analysis revealed increased macroporosity in the porous coatings, while microporosity remained unaffected. Photodegradation of TET followed pseudo-first-order kinetics, with the D32K film achieving an initial reaction rate of 178.46×10^{-6} $mol_{TET} \cdot m^{-2} \cdot L^{-1} \cdot min^{-1}$, more than double that of the non-porous film (78.12×10^{-6} $mol_{TET} \cdot m^{-2} \cdot L^{-1} \cdot min^{-1}$). In terms of reusability, D32K maintained high efficiency over three consecutive 300-minute cycles, reaching an average conversion of 99.8%, compared to 98.6% for the non-porous film. This marks a notable improvement over previous results (87% conversion)[2]. Final

mineralization levels were 96.1% for D32K and 91.7% for the non-porous counterpart. Differences in degradation pathways were observed, as the m/z 431 intermediate, detected in the non-porous film, was absent in the D32K reaction mixture.

Acknowledgements

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The New Particle Formation at Two Heights: Instrumental Comparison

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Atmospheric aerosols significantly affect human health, climate, radiation balance, or visibility. They get to the atmosphere directly, or form from gaseous precursors. During the latter, molecules cluster and grow into aerosol particles. These clusters typically form in the morning and either grow, stabilize, form larger particles (New Particle Formation, NPF) or vanish. The mechanisms driving it are still not fully understood. NPF events are influenced by various environmental factors.[1] Only a limited number of instruments can detect the smallest particles, around 1 nm in diameter, at the very start of NPF events.[2]

In this study, particle formation and subsequent growth are investigated through particle and/or cluster concentration measurements. The measurements are conducted at the rural background site National Atmospheric Observatory Košetice (NAOK, 49.5727367N, 15.0798175E). A 250-meter-high atmospheric tower allows measurements at various heights, from the ground level up to 230 meters above the ground level (a. g. l.).

Various instruments are used there (Tab. 1) to measure particle size distribution. The data from the two different heights are to be evaluated and compared. The meteorological and other parameters affecting the NPF are monitored.

A method for combining the data from the devices mentioned above must be developed since each device works on a different physical principle. Obtaining data from different devices and obtaining a time evolution of the merged particle size distribution helps us picture the NPF from the beginning and better understand its principles.

The first experimental campaign compared PSM and NAIS by measuring the monodisperse aerosol in the Prague Center for Aerosol in Situ (PACC). The second experiment compared the data from PSM, NAIS, and nanoSMPS placed at the NAOK observatory's ground level.

Tab. 1: The list of devices used and their placement

Device	Device Range	Manufacturer
Ground level		
PSM (Particle Size Magnifier)	1–12 nm	Airmodus, Finland
NAIS (Neutral and Air Ion Spectrometer)	0,8–40 nm	Airel, Estonia
SMPS (Scanning Mobility Particle Sizer)	10–800 nm	TSI, USA
Tower, 230 m a. g. l.		
nanoSMPS (nano SMPS)	1,2–40 nm	TSI, USA
NAIS (Neutral and Air Ion Spectrometer)	0,8–40 nm	Airel, Estonia
SMPS (Scanning Mobility Particle Sizer)	10–800 nm	TSI, USA

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Catalysts of Heteroatom Elimination in the Refining of Hydrocarbon Feeds

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Heteroatoms N, O, S, or Cl bound in hydrocarbons represent a barrier in the chemical processing of fossil and renewable feeds. They are removed by various decomposition reactions. For example, hydrodeoxygenation (HDO) is used to eliminate oxygen in biomass-based feeds such as triglycerides containing long hydrocarbon chains. HDO, however, is not convenient for feedstocks rich in oxygen such as saccharides or bioalcohols because it consumes an unacceptable amount of H_2. Dehydration of such feeds to produce olefins appears more attractive despite the need of subsequent oligomerization. Dehydration of bioalcohols, however, can be accompanied with carbon-carbon condensation reactions to yield high-value hydrocarbon derivatives. Low activity of solid catalysts in C-C condensation limits large-scale industrial implication. The C-C condensation includes the Guerbet coupling, direct coupling and formation of $2n-1$ and $2n$ ketones. We investigated Li, Na, K, Mg, Ca, Sr, Ba, Sc, Y, La, Ce, Sm, Eu, Co, Ni, and Cu oxides supported on activated carbon (0.6 mmol g^{-1}) in the reaction of 1-butanol in a fixed-bed tube reactor at 400 °C and atm. pressure. We found that Li and Mg exhibited the highest C-C condensation activities within the studied alkaline and alkaline earth metal oxides, respectively, possessing pseudo-first-order rate constant, k_{C-C}, of the formation of condensed C_7+C_8 hydrocarbons and hydrocarbon derivatives 200 and 160 mg $g^{-1}h^{-1}$. Moreover, La and Sm oxides led to the highest activity within all studied oxides possessing k_{C-C} 420 and 470 mg $g^{-1}h^{-1}$, respectively. In contrast, only toluene and methane were found over Co and Ni oxides despite total conversion of 1-butanol. The supported Mg species were most selective to Guerbet coupling ($2n$ pathway) and to the formation of C_8 derivatives. The ratio of pseudo first order rate constants k_{C8} (the formation of all C_8, the $2n$ pathways) to k_{C7} (the formation of all C_7,

the *2n−1* pathway, mostly 4-heptanone) was 1.9. In contrast, the high activity of the Li, La, and Sm counterparts was accompanied with high selectivity to C_7 providing the k_{C8}/k_{C7} ratio 0.9, 0.4, and 0.4, respectively. The most active Mg, La, and Sm catalysts were also investigated at the 2.5-40.0 wt.% oxide loading range. The increasing activity k_{C-C} was observed with the increasing loading up to about 10 wt.% for the MgO and 25 wt.% for the La_2O_3 and Sm_2O_3. Then, the k_{C-C} leveled off at the values about 210 and 1000 mg $g^{-1}h^{-1}$, respectively. The selectivity index k_{C8}/k_{C7} was hardly influenced by the studied loadings. The investigation into prolonged (5 days continuously) reaction of ethanol over 30 wt.% MgO, La_2O_3 and Sm_2O_3 catalysts showed that the yields of butanols (*2n* pathways) were 6.3, 5.8 and 5.0 wt.% while the yields of acetone and isopropanol (*2n−1* pathway) were 0.9, 3.5 and 5.5 wt.% respectively, at the conversions of ethanol 20, 25, and 30%, respectively. We concluded that the C-C condensation reaction of 1-butanol and ethanol over the studied catalysts proceeded in a similar way. The high activity in total C-C condensation is accompanied with high selectivity to *2n−1* pathway, i.e. to the formation of symmetrical ketones. Low yields of the coupled *2n* alcohols or aldehydes are caused by subsequent C-C coupling or dehydration reactions. The studied bioalcohol reactions provide a promising and sustainable alternative to conventional petroleum processing.

DBSCAN Application for Bubble Tracking in Aerated Columns

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Bubble dynamics significantly affects the performance of multiphase reactors and has an impact on mass transfer, intensity of mixing and overall reactor efficiency. Knowledge of the motion trajectory and properties of bubbles in these systems enables optimization of industrial processes. The aim of this work was to develop an optimal methodology for bubble trajectory tracking based on post-image processing data analysis using the DBSCAN (Density-Based Spatial Clustering of Applications with Noise) algorithm[1]. The focus was placed on identifying suitable DBSCAN parameters to ensure accurate trajectory reconstruction, minimizing both the loss of relevant data and the incorrect merging of separate bubble paths. The methodology was then validated using experimental data obtained from high-speed imaging of a bubble column.

In this work, DBSCAN is used not for general clustering, but specifically to reconstruct individual bubble trajectories by grouping spatially and temporally related position data. Each trajectory is formed as a separate cluster based on the density of detected bubble positions in space (2D) and time. The algorithm does not require prior knowledge of the number of trajectories and can adapt to the irregular motion typical for bubbles in gas–liquid systems.

The results demonstrate that the DBSCAN method successfully differentiates individual Bubble paths and enables the study of their properties in motion. This approach provides a reliable and automated method for bubble tracking in high-speed capturing experiments.

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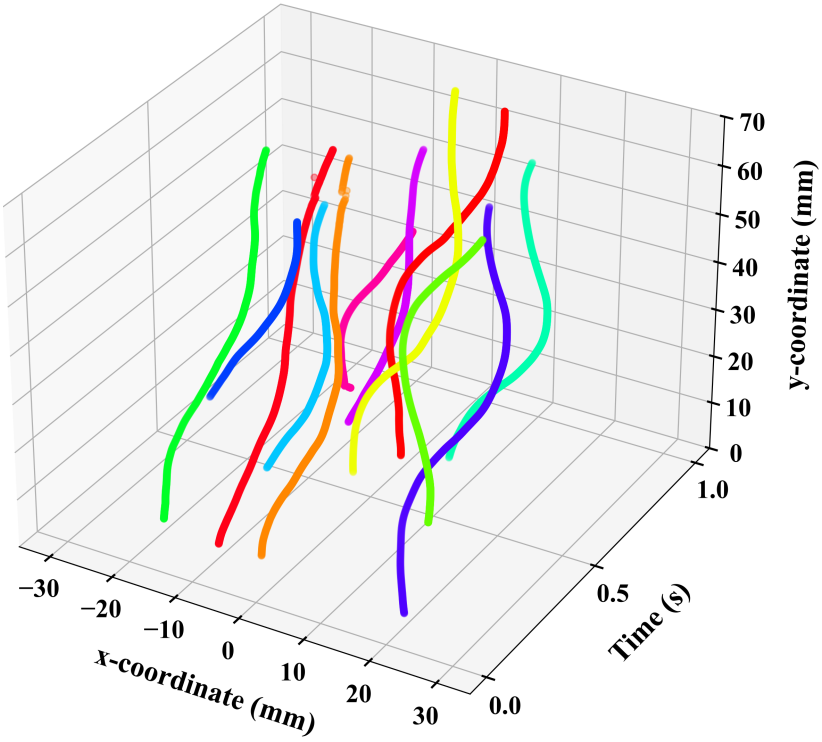

Figure 1: Example of the resulting trajectories of individual bubbles detected by DBSCAN.

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The Effect of Friction Coefficient on the Process of Segregation in a Vertical Bladed Mixer

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Granular materials are ubiquitous in nature and industry, with more than half of global processes involving them at some stage. However, controlling these materials remains challenging, particularly when unwanted particle segregation occurs during processing. Understanding granular dynamics is therefore crucial—not only for optimizing industrial operations but also for explaining natural phenomena such as avalanches, landslides, and planetary ring formation. In recent decades, significant advancements in segregation research have been made through both experimental and computational approaches, especially via the Discrete Element Method (DEM).

Segregation arises from differences in particle density, size, surface roughness, and frictional interactions. Despite identifying multiple segregation mechanisms, a comprehensive theoretical framework remains elusive[1,2]. This study investigates the impact of varying the particle–particle friction coefficient (ranging from 0.1 to 0.9) on segregation in a binary granular mixture. DEM simulations were conducted in a vertical cylindrical mixer equipped with dual-bladed stirrers pitched at 45°, operating at 150 rpm. The system included 36,800 particles (2 mm) and 400 particles (4 mm); the larger particles were initially placed either at the top or bottom of the bed.

Experimental validation confirmed the consistency of simulation results. Analysis revealed that, after sufficiently long mixing, the initial placement of larger particles had minimal influence on final distribution; instead, secondary flows emerged as the predominant factor governing segregation. Higher friction coefficients led to more intense recirculation zones and flow patterns. Several characteristic behavior patterns of large particles were identified that determine whether segregation occurs or not. An in-depth analysis of average particle motion confirmed that, after prolonged mixing, final particle distribution is governed primarily by interparticle friction, rather than initial configuration. These findings contribute to a deeper understanding of segregation mechanisms in granular systems and their potential impact on industrial processes.

Acknowledgements

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Enantiomeric Separation via Chiral Membranes and the Effect of a Magnetic Field

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Enantiomers have the same physicochemical properties in an achiral environment. They are mirror images of each other, similarly to our left and right hands. Chirality in nature occurs in many life-important compounds, such as amino acids, carbohydrates, steroids and alkaloids. Chiral compounds can drastically impact our health, as in some drugs both enantiomers might be present and could have very different therapeutic effects in our body. One of enantiomers can be curative, while the other can be inactive or, even worse, harmful. Examples of chiral drugs are Ibuprofen, Cetirizine or Penicillamine. It is, however, not always possible or economical to produce enantiomerically pure drugs via asymmetrical synthesis. The other approach, separation of the racemic mixtures, is still challenging due to the nearly identical molecular structure of the enantiomers and difficulties with finding a suitable system of chiral selectors and experimental conditions (solvent, pH, temperature, etc.). Currently used separation techniques involve capillary electrophoresis, preferential crystallization or high-performance liquid chromatography (HPLC), but they have limited applicability.

Our approach is to develop enantioselective membranes, potentially offering scalable technology for continuous or semi-continuous processing. Adding the effect of the homogenous magnetic field to the separation process is promising to enhance enantioseparation with other physical means at the molecular level[1]. Radical derivatives of amino acids are used for separation with a magnetic field. In my case, it is radical TEMPO-tryptophan in zwitterionic form. Membranes are prepared in collaboration with the nanotechnology group at the Technical University in Liberec. These composite mem-

branes contain a nonselective nanofiber support with paramagnetic nanoparticles of iron and a thin layer with chiral selectors prepared by interfacial polymerization. The chiral selector is based on (S,S)-1,2-diaminocyclohexane, which was proven to separate tryptophan in an aqueous environment[2]. We further created a magnetic-field-responsive chiral membrane by modifying the commercial ionomer Nafion with gadolinium and an organic chiral ligand based on mandelic acid. This membrane is also suitable for separating enantiomers of tryptophan. Gadolinium ions were chosen due to their ferromagnetic properties to enhance the action of a magnetic field close to the active site of the chiral selector.

Acknowledgements

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Cultivation Conditions Optimization for *Galdieria sulphuraria* Biomass and Phycocyanin Production Maximization

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Galdieria sulphuraria is a polyextremophilic red microalga, one of the few eukaryotic species capable of phycocyanin (PC) biosynthesis. It has recently been proposed as a food-grade, acid tolerant production vector for PC and glycogen, due to its ability to thrive at conditions considered lethal for the vast majority of mesophilic contaminants, while maintaining relatively high productivity[1]. Unlike the PC commonly derived from *Arthrospira sp.*, PC sourced from *Galdieria sp.* displays greater stability at high temperatures and low pH, making it a suitable food colorant for food and beverage applications. Although the individual optima for photoautotrophic cultivation temperature and pH are already known, their coupled effect on the cultivation productivity and intracellular PC accumulation is yet to be determined [2]. This study aims to generate a robust dataset describing the interplay between pH and temperature on the growth and PC biosynthesis of *Galdieria sulphuraria*, utilizing a central composite design of experiment. Data interpolation was utilized to generate discrete surface response models, displaying that the conditions for maximized intracellular PC content deviate from those which maximize biomass productivity. Our results provide a comprehensive insight into the cultivation conditions optimization for phototrophic *Galdieria sp.* cultivation, and demonstrates its potential for targeted pigment or biomass production in indoor photobioreactor systems.

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Phosphorus-derived Phenanthrenes: Synthesis and Properties

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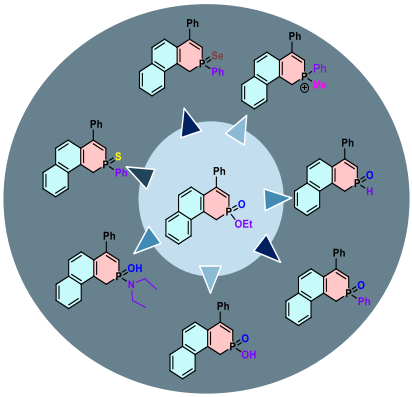
Polycyclic aromatic hydrocarbons (PAHs), which are organic compounds composed of two or more fused benzene rings, play a significant role in optoelectronic devices due to their unique optical and electronic properties. They are particularly useful as building blocks in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs), and other optoelectronic devices. However, these polycyclic aromatic hydrocarbons usually lack certain necessary features and often require optimization to fulfill the requirements.[1] One of the main strategies used is the incorporation of a heavy atom into polycyclic aromatic systems. Among the other elements, that have been discussed in the literature, the phosphorus atom is not so common, especially when it's incorporated into a hexacycle.[2]

An incorporated phosphorus atom can significantly improve the solubility, stability or modify optical properties of the original compound and once present, it can be easily tuned via various derivati-



zation reactions. These "on-phosphorus post-functionalization" processes are a powerful tool for studying the impact on the molecular properties.[3]

In this study a series of stable polycyclic aromatic systems containing six-membered phosphorus cycle are prepared, using the post-functionalization strategy. The influence of the derivatization on chemical and physical properties is then discussed.

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Cloud Droplet Formation: The Crucial Role of Cloud Condensation Nuclei

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Atmospheric aerosol particles serving as cloud condensation nuclei (CCN) are important components of the hydrological cycle and climate due to their influence on cloud microphysical structures and radiative properties.[1] Their indirect effect on the radiative balance of the atmosphere, through changes in cloud droplet number and persistence, represents the largest uncertainty among the currently known drivers of radiative forcing.[2] CCN closure studies, which compare predicted and measured CCN number concentrations using aerosol properties and hygroscopicity parameter (κ), derived from Köhler theory, are commonly used to assess current knowledge and often achieve agreement under background atmospheric conditions with low pollution levels.[3]

This study investigates aerosol hygroscopicity and CCN activation ratios using aerosol size distribution, chemical composition, and meteorology measured at the National Atmospheric Observatory Košetice, Czech Republic. The study findings showed that CCN activation ratios (AR) increase with increasing supersaturation (SS) across all clusters of air masses, as expected. Higher SS allows a broader range of particle sizes and compositions to activate into cloud droplets. However, at low SS (0.1–0.3%), clusters originating from the Atlantic region exhibit slightly higher AR, while Eastern European clusters show the lowest activation efficiency. This suggests that particles from Eastern Europe are less hygroscopic or smaller, requiring higher SS to activate. In contrast, oceanic air masses contain more hygroscopic aerosol species, such as sulfates and ammonium, which activate more readily at lower SS. At higher SS (0.5 to 1.0%), the differences among clusters become less pronounced, as more particles across all sizes and compositions reach activation thresholds. Nonetheless, oceanic air masses still trend slightly higher in activation efficiency. In conclusion, the

observed trends underscore the importance of regional source characteristics in shaping aerosol-cloud interactions, which are critical for understanding cloud formation processes and their impact on climate.

Acknowledgements

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Tracing Airborne Pollutants: Investigating Metals in Atmospheric Aerosols

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Particulate matter (PM) in the atmosphere and its chemical composition are the subject of detailed study worldwide due to their significant impacts on human health, the environment, and climate[1]. Metals are integral components of the atmospheric PM, originating from both natural and anthropogenic sources [2]. Recent studies also highlight the role of metals as effective markers for identifying specific pollution sources[3].

This study aims to investigate the presence, sources and transport of metallic elements in atmospheric aerosols, with a particular emphasis on temporal (seasonal and diurnal) variability of metals in particulate matter (PM) and identify their emission sources. The cutting-edge X-ray fluorescence (XRF) spectroscopy (Cooper Environmental Xact 625i, ElvaX PMX) will be utilized for near real-time metal analysis with superior time resolution and simultaneous multi-element detection, which facilitates the examination of swift changes in metal levels and enhances source apportionment. The measurements will take place at a rural background site, National Atmospheric Observatory Košetice and an urban background site at Suchdol, Prague, Czech Republic. By integrating XRF and meteorological data, we aim to understand the physico-chemical properties and atmospheric behaviour of metal-containing aerosols and improve knowledge of their sources.

Along with the online analytical methods, offline method of PM sampling using a Davis Rotating-drum Uniform-size-cut Monitor — 3DRUM (DELTA Group, UC-Davis)[4] will be utilized, followed by chemical characterisation of samples, for better comprehensibility.

Acknowledgements

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Ice Nucleation Particles in the Central European Atmosphere

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Ice Nucleation Particles (INP) are essential in cloud formation processes and properties. They modify the cloud's albedo, lifetime, and precipitation. The amount of data for direct INP measurements is still very low, while clouds are one of the most complex phenomena in climate and weather studies. We aim to use a Portable Ice Nucleation Experiment (PINE)[1] to measure directly INP with a frequency of 10 minutes during a one-year-long measurement campaign at two different sites. The first site is the National Atmospheric Observatory Košetice (NAOK), representing rural background areas of central Europe, and Milešovka, a remote measurement site north of Prague, allowing cloud in situ measurement. New INP parameterizations will be derived from the measurements to retrieve INP from simpler, more widely available aerosol measurements, and compared for the two different environments.

In parallel with the installation of PINE, some preliminary analyses on INP concentration are done thanks to previous parameterization, based on the number of aerosols larger than 0.5 μm in diameter[2]. The data account for 1263 h, a total of 48 full days of measurements at NAOK at 230 m above the ground. When comparing INP concentration for periods within and above the Planetary Boundary Layer (PBL) height, we find significantly higher concentrations (based on the Mann-Whitney U test) for all mixed-phase cloud temperature ranges when the measurements are within the PBL (Figure 1).

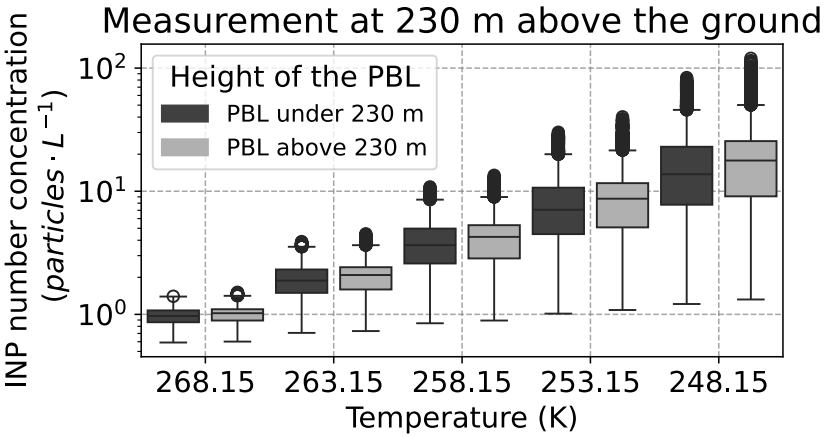

Figure 1: Box plot of INP number concentration retrieved from DeMott et al (2010) parameterization for different freezing temperatures.

Acknowledgements

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