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## **Exploring Bubble Dynamics with VOF Method Simulations: Insights from Two Fundamental Gas-Liquid Flow Case Studies**

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**INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS OF THE CAS**

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# Development of Polymeric Enantioselective Membranes

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Enantiomers are molecules that share the same chemical formula but in space form mirror images of each other. Their reactions with other chiral molecules can be remarkably different, which is crucial mainly for pharmaceuticals and agrochemicals. However, industrial-scale synthetic production of enantiomerically pure compounds is not always available. Therefore, the need for pure enantiomeric compounds drives the development and research on various separation methods. However, most methods used on the industrial scale are limited to specific compounds (diastereomeric recrystallization) or generally difficult and/or expensive to scale up (chromatography-related methods). Separation of enantiomers using membranes is promising thanks to the easy scalability and continuous operation of membrane processes. Various ideas about how the enantioselective membranes should look like have been published in the last thirty years. The mechanism of enantiomeric separation on a membrane is, however, highly specific, and still requires extensive research.

In this work, four types of enantioselective polymeric membranes are presented. The first type consists of inherently chiral polyimide synthesized from chiral precursors<sup>1</sup>, that was combined with film-forming polymers Matrimid®, ethylene-co-vinyl alcohol (EVAL™) and poly(ether-block-amide) (PEBAX®1657) to obtain a self-standing or composite membrane. Generally, there is a trade-off between the mechanical stability and permeability of the prepared films, which also compromises the potential selectivity. The second type presents a simple way of mixed-matrix membrane preparation by mixing  $\beta$ -cyclodextrin as a chiral selector with EVAL™ polymer. Although the loading of the membrane with the selector can be as high as 50 wt. %, enantioselectivity for selected enantiomers was not detected, probably due to the blockage of the chiral centers by the polymer. Within the third type, an ionic interaction between a charged membrane and an oppositely charged chiral selector based on ionic liquid or  $\beta$ -cyclodextrin derivative was used to prepare modular chiral

membranes using the dip-coating method. It is shown that the membranes based on anionic  $\beta$ -cyclodextrin derivative are selective towards N-Boc-tryptophan and, based on the parametric study presented, the separation mechanism can be described as sorption-selective. Finally, the fourth type explores the chiral ion exchangers as the selectors in enantioselective membranes<sup>2</sup>. Separation of N-(3,5-Dinitrobenzoyl) leucine enantiomers on a new mixed-matrix cation exchange enantioselective membrane reveals that controlling the ion-displacement mechanism is crucial to the separation efficiency. We detected the enantiomeric excess as high as 90% in permeate but it decreased in time. Outcomes and prospects of the individual types of enantioselective membranes are discussed.

#### *Acknowledgements*

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# Emerging Contaminants in Sewage Sludge: Analysis and Their Removal by Pyrolysis

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Sewage sludge, along with organic matter, contains a variety of emerging pollutants, such as per- and polyfluoroalkyl substances (PFASs) or flame retardants, which complicate their material use<sup>1</sup>. Their removal from the sludge matrix is necessary to avoid contamination of the environment or harm to human health. Our previous work showed that PFASs present in sewage sludge can be removed by pyrolysis above 400 °C<sup>2</sup>. These results were verified and confirmed by analysis on a commercial pyrolysis unit at the Bohuslavice-Trutnov WWTP, operated at 600 °C. For validation, an analysis of organic fluorine (part of the PFASs molecule) was included to demonstrate that PFASs were removed and no degradation to organofluorine substances and other non-analysed PFASs occurred. The results of the organofluorine analysis confirmed that above 400 °C, organofluorine is removed from the solid matrix (sludge-char), but organic fluorine is part of the primary pyrolysis gas<sup>2</sup>. The study continues with flame retardants (e.g., phosphorus-based or brominated) present in sludge, which may pose a hazard to nature and human health<sup>3,4</sup>. There is a lack of information on their pyrolysis removal and occurrence in the sludge in the Czech Republic. Based on a screening test of sludges originating at WWTPs with full-scale sludge drier installation, we selected the sludge with the highest representation and abundance of flame retardants, which was further pyrolysed at 200–700 °C to determine the minimum temperature for their removal. In addition, the initial results at the commercial pyrolysis unit at the Bohuslavice-Trutnov WWTP show the removal of 85% of the original amount at 600 °C.

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# Assessment of the Presence of Hazardous Components in Textile Waste

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The textile industry is of global importance as a provider of products for human comfort. However, the textile value chain is long and complex, with a number of process steps that use large quantities of a variety of chemicals. Many of these chemicals have toxic and ecotoxic effects not only during production but also at the end of their life cycle. Among the most problematic substances are dyes and pigments, most of which consist of synthetic organic compounds and contain heavy metals that are known to persist and bioaccumulate in the environment<sup>1</sup>. Another group of hazardous substances are per- and polyfluorinated alkyl substances (PFAS), which are widely used in textile products as part of repellents due to their excellent hydrophobic and oleophobic properties<sup>2</sup>. These are also toxic, persistent and highly bioaccumulative. With the number of chemicals used in textiles increasing daily, there is still a lack of safety information on the presence and use of all these chemicals, which is currently a major research gap. Identifying potentially toxic compounds in textile waste through laboratory testing is therefore the aim of our key research.

An up-flow percolation test was chosen to identify and characterize heavy metals and PFAS constituents in textile waste. Up-flow column percolation tests are used on a laboratory scale to assess the leaching behavior of a hazardous substance from a waste in a given state as a function of time. The test was performed according to the European Technical Standard CEN/TS 14405. Preliminary results showed the following heavy metals in the leachates Al, As, Co, Cr, Cu, Fe, Mn, Pb, Zn and Sb, with Al, Cr, Fe, Mn and Zn being predominant. For example, Al is used as an additive in firefighting suits and protective clothing for its antistatic properties and ability to reflect radiant heat and electromagnetic radiation. Cr, Fe, Mn are used to dye fibers. Zinc oxide is applied to woven and knitted cotton fabrics to protect human

skin from UV radiation. Trace levels of perfluorooctanoic acid (PFOA), perfluorononanoic acid (PFNA), perfluorodecanoic acid (PFDA) and 8:2 fluorotelomer sulfonate, which are used as surfactants in the textile industry, were also found in the leachates above the detection limit.

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# Multi-Annual Characterization of PM1 Aerosol Optical Properties and Size Distribution at the Peri-Urban Atmospheric Site ATOLL in Lille

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The aim of this study is to present aerosol scattering, absorption properties and particle number size distribution in PM1 in years 2018-2022 at peri-urban atmospheric site "Atmospheric Observations in LiLLe" (ATOLL) in Lille, France. This study is the first to present results dedicated to aerosol scattering properties at this site.

The Mann-Kendall seasonal test showed a significant decrease of total scattering coefficient  $\sigma_{sp}$  at 525 and 635 nm over time, both decreased by  $2.0 \text{ Mm}^{-1}/\text{year}$ , respectively. No significant decrease was observed for backscattering coefficient  $\sigma_{bsp}$  at any wavelength, suggesting an increase in the backscatter fraction relative to total scattering.

The median absorption coefficient  $\sigma_{ap}$  at 525 nm was  $5.1 \text{ Mm}^{-1}$ , the median conc. of eBC at 880 nm was  $330 \text{ ng m}^{-3}$  and the median conc. of BrC at 370 nm was  $100 \text{ ng/m}^3$  throughout the period. A significant decrease of  $0.3 \text{ Mm}^{-1}/\text{year}$  was observed for  $\sigma_{ap,ff}$  suggesting a continuous reduction of fossil fuels detected at the site over time.

The particle number size distribution was divided into 20–30 nm, 30–300 nm and 300–800 nm modes with conc. of 1216, 4268 and 43 particles/ccm<sup>1</sup>, respectively. The significant increase in conc. was observed in 20–30 nm and 30–300 nm modes by 239 and 317 particles/ccm/year, respectively. Based on Crumeyrolle et al. (2023)<sup>1</sup>, who observed a strong influence of new particle formation events on the number conc. from 15.7 to 100 nm in summer and spring at ATOLL site, further investigation will be performed to link NPF frequency with the significant increase in particle concentration in 20–30 nm size mode at the site.

The conflict in Ukraine led to restrictions on Russian gas supply to Europe, resulting in a European oil and gas crisis in 2022. The signif-

icant increase in almost all measured aerosol properties was observed in December 2022, hypothetically due to the use of different sources for energy production. Additional analysis of the chemical composition showed three episodes of substantial increase of sulphate, nitrate, and OM concentration in December 2022, considering potential partial return to coal combustion. Analysis of HYSPLIT ten-day backward trajectories in December 2022 of the episodes indicated Central and Eastern Europe, the UK and local sources as the main contributors to the increased levels of aerosol properties in December 2022.

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# Development of Continuous Technology for the Preparation of Pharmaceuticals

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Transition of a batch synthesis to continuous process in pharmaceutical industry is an intensively studied theme in the last years. Many successful approaches to transition of the reactions into flow process<sup>1</sup> have been published. The present research focuses on the transition of a batch reaction assisted by phase transfer catalyst (PTC) into continuous process. The first reaction studied was an N-alkylation reaction with methyl ester of the 1-methyl-10 $\alpha$ -methoxydihydrolysergic acid (MeLUME) as product. MeLUME is one of the intermediates in synthesis of drug Nicergoline. The N-alkylation occurs in two different immiscible phases and the bridge between these phases is the phase transfer catalyst. The study was performed in several different continuous flow apparatuses. The best results were obtained in a capillary reactor, with assistance of ultrasound. It is supposed that the application of ultrasound increases the surface area of the dispersed phase by breaking it into smaller droplets and hence facilitating the mass transfer through the phase interface<sup>2,3</sup>. It was possible to measure the reaction kinetics in the capillary reactor. In line with the literature, we concluded that the deprotonation step of the N-alkylation is the reaction determining step. Based on these steps we designed a kinetic model.

Based on the results obtained, a new objective was set to verify the applicability of the knowledge gained in the study in order to develop general approaches for the continualization and intensification of organic syntheses containing PCT reactions. The second reaction chosen is the synthesis of a drug Trazodone. Trazodone can be used as an antidepressant or hypnotic. One of the approaches for continuous system was described by Jaśkowska et. al<sup>4</sup>, while the synthesis is carried out in two steps with ultrasound assistance. In contrast to firstly studied N-alkylation with liquid–liquid phase system, the synthesis of Tra-

zodone is carried out at a solid–liquid interface. The hypothesis for the reaction intensification with solid–liquid arrangement is that the sonication accelerates the transport from the surface of the solid to the organic phase and thus it intensifies the reaction.

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# Drone Based Vertical Profiling of Black Carbon Aerosols at a Rural Background and an Urban Site in Central Europe

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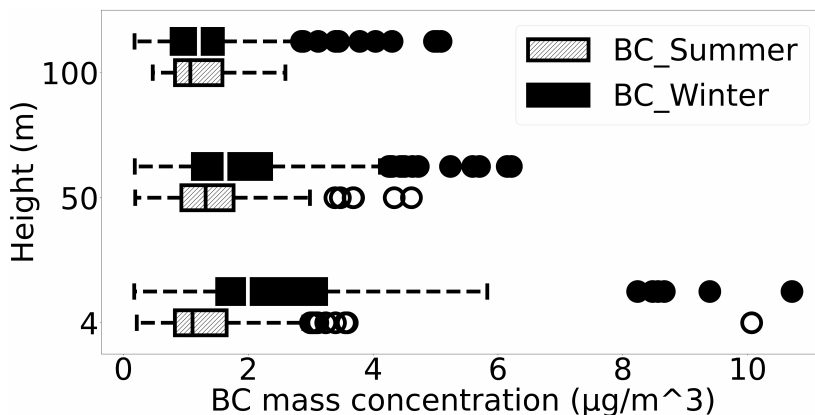
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Black Carbon (BC) aerosols are primary particles emitted into the atmosphere as a by-product of incomplete combustion processes (Bond et al., 2013). The Earth's radiative properties are strongly influenced by vertical distribution of BC (Haywood and Ramaswamy, 1998) and thus the understanding of the vertical distribution of BC is crucial for accurately assessing the BC impact on climate systems.

This research aims to assess the vertical distribution of BC aerosols using a drone and micro Aethalometer AE51 at two distinct sites in the Czech Republic: 1. NAOK (National Atmospheric Observatory



Košetice) representing a regional background, and 2. MFF (Faculty of Mathematics and Physics in Prague) representing an urban site. At NAOK, a 250-meter measurement tower is accessible, providing a means to validate and calibrate the drone measurements.

During summer, BC concentrations exhibited relatively consistent vertical distributions in the lowest 100 meters, while a noticeable decrease in concentrations with height was observed during winter (Figure 1). The influence of a stable atmosphere on vertical profiling was evident: by inhibiting vertical mixing it effectively trapped pollutants near the surface. Additionally, the entrapment of pollutants was closely associated with the height and strength of temperature inversions, significantly influencing the vertical dispersion pattern. BC concentrations increased during winter by 100%, 45%, and 18% at 4 m, 50 m, and 100 m, respectively, compared to the summer (Figure 1) at MFF.

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# Growth and Phosphorus Dynamics During *Tolypothrix tenuis* Cultivation – a Cyanobacterium of Biotechnological Potential

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So called “luxury phosphorus uptake” (LPU) is one of the most advantageous evolutionary features of cyanobacteria and algae. Some algae, when exposed to an environment with excess phosphorus (P), have the ability to assimilate more phosphorus than they actually need for growth and reproduction, and are able to build up a P-stock for future use. This ability is called LPU<sup>1,2</sup>. Since P is the major limiting element upon which the primary production of aquatic ecosystems is based, LPU gives an advantage over other organisms and allows them to increase their biomass rapidly. Here I investigated the course of biomass growth, phosphorus uptake and changes in intracellular phosphorus content in *T. tenuis* in a batch cultivation. Cultivation experiment was held in multiple bubble columns during a light regime (alternating light and dark periods 16 and 8h). Thanks to this experiment I was able to obtain a growth curve of *T. tenuis*. The decrease of phosphorus concentration in the medium was disproportionally faster than biomass growth resulting in significant oscillations of phosphorus content in the biomass, which are typical characteristics for LPU. It was also observed, that after all phosphorus was removed from the medium, the algae growth continues over time, while obviously utilizing intracellular phosphorus reserves. These findings are valuable in course of using this cyanobacterium for efficient bioremediation of eutrophic water based on phosphorus removal by targeted algae cultivation.

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# **Cholinium Based Ionic Liquids: Influence of Water as a Co-solvent on Their Physico-chemical Properties and Preliminary Results for Dissolution of Biopolymers**

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Ionic liquids (ILs) are emerging as promising alternative solvents in the field of natural substance extraction, offering significant advantages<sup>1</sup> over traditional solvents. Since the last decade, we notice the increasing use of greener solvent alternatives such as Natural Deep Eutectic Solvents (NaDES) or ILs for the extraction of highly valuable compounds from natural sources such as lignocellulose<sup>2</sup>. The crucial issue of the dissolution of lignin, a complex and resistant polymer, is being explored in the context of biomass and waste recovery.<sup>3</sup> The efficient dissolution of lignin in ILs offers opportunities for its valorization, leading to the development of new pathways for transforming lignocellulosic biomass into chemicals, biofuels and advanced materials.<sup>4</sup> Moreover, the extraction of lignin, an abundant by-product of the paper and biomass industry,<sup>5</sup> is an area of particular interest.

ILs exhibit unique properties such as their high thermal stability, low volatility, and ability to dissolve a wide range of organic and inorganic compounds. These characteristics make ILs attractive candidates for the selective extraction of bioactive compounds from renewable feedstocks.

Understanding their physicochemical properties are crucial for designing them as a tool to optimize their use. During this presentation, the influence of water on heat capacity, density, speed of sound and TGA will be discussed and the preliminary results for lignin dissolution will be presented.

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# Vertical Gradients of Atmospheric Aerosols Chemical Composition

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In spite of recent considerable progress, the understanding of atmospheric aerosol (AA) sources, chemical composition (CC), transformation processes and environmental effects is limited.<sup>1</sup>

Mass spectrometry of AA has become the most essential and fastest growing area of aerosol research.<sup>2</sup> Aerosol Mass Spectrometer (AMS) is widely used to determine the concentrations of chemical species in AA particles. Followed data analysis deconvolves the ensemble mass spectrum into the partial spectra of distinct chemical species.<sup>3</sup>

Investigating vertical gradient of AACC by studying characteristic mass to charge ratio ( $m/z$ ) of ionisation fragments of AA chemical constituents is a novel approach that has not yet been used. Also, the 250 m tall tower installation for AA sampling at National Atmospheric Observatory in Košetice (NAOK) is unique in the Czech Republic. Moreover, these kinds of installations are scarce even globally. NAOK is a reference rural background site which offers insight into comparison of AACC from local sources and those from long-range transport.

Two sampling routes connected to the AMS (230 m long tube from the tower and 4 m above ground) are being switched regularly in given intervals (15 min).

It is known that aerosols collected at the ground level originate mostly from local sources, typically residential heating, agriculture and traffic. In Košetice area, there are no major industrial sources of AA. Aerosols at a higher altitude are long-range transported (typically aged continental, marine and originated from forest fires and volcanic eruptions).<sup>4</sup>

The organic ions are associated with several types of organics including mass spectral markers for hydrocarbon-like ( $m/z$  57) and oxygenated ( $m/z$  44) organics.<sup>5</sup> Some of the other characteristic ionization

fragments are ethyl ion ( $m/z$  29), propyl ions ( $m/z$  43), markers of burning ( $m/z$  55 and 91), biomass burning specifically (e.g. levoglucosane) ( $m/z$  60 and 73) or polyaromatic hydrocarbons (PAH) ( $m/z$  173).

Concentration of chemical species chosen as markers for AA source apportionment are evaluated with regard to atmospheric conditions, seasonal and daily cycles and compared between the two heights. This work adds to the current state of general knowledge about AACC.

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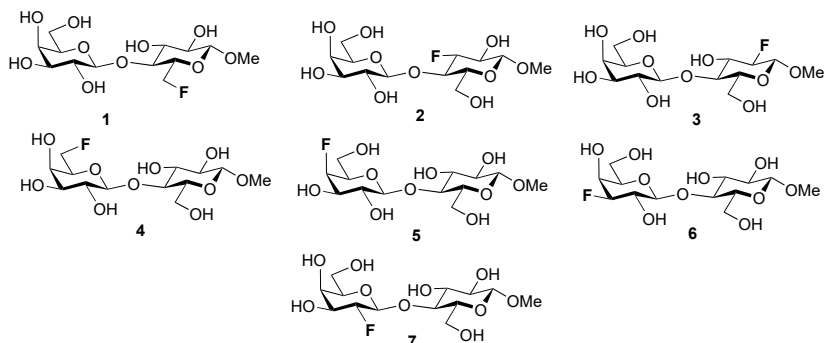
# Synthesis of Fluorinated Methyl $\beta$ -Lactosides

Student: Ing. Aleš Krčil

Supervisor: Mgr. Jindřich Karban Ph. D.

Human galectins (*hgals*) are carbohydrate-binding proteins that have the ability to regulate immune responses and processes related to neoplastic transformation by recognizing galactoside-containing glycans.<sup>1</sup> Consequently, there has been a growing interest in developing selective galectin inhibitors. However, this is challenging due to the existence of 12 *hgals* with similar substrate specificities. A deeper understanding of the distinctions between individual *hgals* could aid in the development of galectin inhibitors. Deoxyfluorinated carbohydrates have at least one hydroxyl group replaced by fluorine, and due to the similarity between fluorine and the hydroxyl group, deoxyfluorinated carbohydrates very well mimic natural carbohydrate ligands.<sup>2</sup> 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  $^{19}\text{F}$  NMR spectroscopy, leading to a more effective description of their molecular mechanism.<sup>3</sup>

In my contribution, I will describe the synthesis of a complete series of mono-deoxyfluorinated methyl  $\beta$ -lactosides (1–7). Their affinity to-



**Figure 1:** Structure of fluorinated methyl  $\beta$ -lactosides.

wards *hgals* will be determined by analytical method ELISA. The synthesis relies on monosaccharide building blocks, which serves as key intermediates that are transformed into the target products through glycosylation followed by final deprotection steps.

#### *Acknowledgements*

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# Investigation of Mechanical Processing of Solar Photovoltaic Panels

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*Supervisor: Ing. Michal Šyc, Ph.D.*

Long-term trends show an increasing solar photovoltaic power plant installed capacity.<sup>1</sup> However, this is also associated with a large production of discarded panels. It is estimated that by 2050 there will be between 60 and 80 million tonnes of waste panels worldwide.<sup>2</sup> Such large amounts of waste could be considered an interesting source of valuable materials. Recycling discarded waste electrical and electronic equipment (including solar photovoltaic panels) is part of what is known as urban mining. This modern way of obtaining resources is focused on metals.

In the case of solar photovoltaic panels, metals are the most valuable part. Particularly, silicon from the silicon cells and wires, made from copper, solder (i.e. lead and tin), and silver. Particularly silver is expected to improve the economic balance of the real-scale process.<sup>3</sup> The less valuable part is glass, which can constitute up to 80% wt. However, at present, the composition of all parts of the panels and suitable technologies on an industrial scale are not well understood and prevent full recycling.

This work aims to describe the possibilities of mechanical treatment of solar photovoltaic panels. In the first part, the shredding and milling process for the transformation of the product (whole panel) into material that can be further processed, was investigated. Milled material was sieved and analyzed. It was observed that this shredding also works as a selective grinding because three main products were produced. The second part of this work was aimed at the physical concentration of silver in real samples of milled solar photovoltaic panels by Knelson separator. This device (type of centrifugal separator) showed the ability to significantly increase the amount of silver in the outcome stream.

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# Cultivation of *Limnospira Maxima* and Utilization of its Fresh Biomass in Human Nutrition

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The dried biomass of the cyanobacteria *L. maxima*, commonly known as spirulina, is a widely available dietary supplement known as a “superfood,” valued for its antioxidants, vitamins, and other nutrients<sup>1</sup>. However, its distinct flavor makes it unattractive for some consumers, and the drying process contributes to increased energy costs<sup>2</sup> and degradation of some of the valuable components during downstream processing. Consequently, certain producers, particularly artisanal ones, are introducing fresh spirulina biomass to the market. With its high-water content (approximately 90% w/w) and protein levels (about 60–70% w/w in dry matter), fresh spirulina is easily spoiled and improper storage practices could pose health risks to consumers<sup>3</sup>. Currently, there’s limited information on the microbiological aspects and storage requirements of fresh spirulina biomass, and there are no specific legal standards in the EU or US. This project aims to fill this gap by presenting new insights into its consumption as an alternative to dried spirulina and offering recommendations for safe storage. The results revealed that fresh spirulina biomass contained no foodborne pathogens. Initial bacterial counts in freshly harvested spirulina biomass were within acceptable limits ( $10^5$  to  $10^7$  CFU/g) and remained stable during the first 16 days of storage at 4 °C. However, bacterial counts increased significantly when the biomass was stored at room temperature (25 °C). Washing the biomass with potable water post-harvest was found to have a negative impact on shelf life at both temperatures tested (4 and 25 °C). Additionally, fresh biomass exhibited higher levels of phycocyanin, carotenoids, and chlorophyll a, compared to dried spirulina. It also boasted more delicate sensory qualities and was better received by consumers. In conclusion, fresh spirulina offers superior sensory attributes and greater health benefits compared to dried spirulina.

However, its shorter shelf life necessitates careful consideration in storage and distribution processes.

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# Axial Dispersion and Mass Transfer in Bubble Column

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*Supervising Expert: Sandra Orvalho, Ph.D.*

Bioreactors find extensive application across various industrial domains, notably within pharmacy and food industry. From the different bioreactor types available, the bubble column stands out as the most suitable for cells sensitive to shear forces. Such cells typically demand precise supply of oxygen. Thus, precise regulation of aeration and homogeneity is crucial, particularly in tall bubble columns characterized by high aspect ratios AR (liquid height to column width). The objective of the study is to experimentally investigate axial dispersion and mass transfer within a bubble column, examining their mutual interrelation and their correlation with operational parameters and AR<sup>1</sup>.

Experiments were conducted in a bubble column with diameter 0.19 meters, gas flow rates varying from 2 to 20 m<sup>3</sup>/h and aspect ratios spanning from 3.0 to 6.0. Gas holdup was measured from changes in surface height with and without aeration. Axial dispersion coefficient  $D_a$  was measured by conductivity method. KCl solution was used as tracer. Three conductivity probes were placed at heights of 43, 83, and 123 cm above gas distributor. KCl concentration profile was fitted by axial dispersion model with  $D_a$  as a fitted parameter. Volumetric mass transfer coefficient  $k_L a$  was measured by Dynamic Pressure Method proved to be one of the most reliable methods<sup>2</sup>.

Obtained results suggest that  $D_a$  considerable increases with liquid height and therefore with AR. Simple empirical correlation predicting  $D_a$  in dependence on AR and  $u_G$  was provided with RSTD 17%. Acquired  $D_a$  values were used in model of mass transfer and data were compared to model assuming ideal mixing of the liquid phase. Results suggest that at low  $u_G$ , the liquid mixing exhibits piston flow, which needs to be considered when modelling the mass transfer. At high  $u_G$ , the liquid mixing can be considered as ideal.

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# Exploring Bubble Dynamics with VOF Method Simulations: Insights from Two Fundamental Gas-Liquid Flow Case Studies

*Student: Mgr. Václav Harrandt*

*Supervisor: Doc. Ing. Jaromír Havlica, Ph.D.*

Four basic constellations of gas and liquid phases, namely bubble, slug, annular, and churn flow regimes, can be encountered in gas-liquid flow in channels<sup>1</sup>. The scientific community should understand such flows, as knowledge of their fundamental behavior is needed in many industrial or energy sectors. This knowledge can help design appropriate operating conditions for devices such as nuclear reactors, heat exchangers, or membrane separation modules.

The interactions between the individual phases are the fundamental predetermining phenomena that subsequently dictate the character of the flow itself. For this reason, it is necessary to deal with the construction of principles that describe these interactions. The present study focuses on the flow of Taylor bubbles, representing the interaction between the channel wall and the gas phase, and the collision of a bubble with a vortex ring, serving as a model liquid-gas interaction. Understanding the former case can be essential to prevent the membrane fouling or the flow induced corrosion. The dynamics of the latter case is the predictive criterion for whether the initial mother bubble will break up into the daughter bubbles or not<sup>2</sup> and this process can therefore be used as an idealized model of turbulent bubble flow.

The current endeavor aims to create a robust simulation cornerstone that, together with experimental investigations, explores the aforementioned issues. The simulations were performed with the OpenFOAM software using the finite volume method for discretization. The Volume of Fluid (VOF) method was used to perform the multiphase flow simulations. In the case of Taylor bubbles, rectangular channels with higher aspect ratio values have been studied, which remains a challenge to this day. An efficient procedure has been implemented that allows the simulation of Taylor bubbles in a moving reference frame, which causes the bubble to remain in an almost static position with respect to the domain. The experiments for this topic were performed using a Plexiglas channel with modifiable geometry, and the bubble motion was recorded using a high-speed camera. The

primary parameters studied included bubble velocity and liquid film thickness for different channel inclinations and geometries. In the case of bubbles interacting with the vortex structure, the experiment required a bubble generator in the form of a capillary and a vortex ring generator consisting of a nozzle connected to a pressurized vessel. The interaction process was recorded by high-speed cameras and complemented by the PIV method to evaluate the velocity field in the plane. The main advantage of simulations is that the results can be evaluated in 3D space, and the obtained results have a better resolution. Therefore, the numerical simulations carried out extend the insight into the secrets of the ongoing processes. Attention has been paid to quantities characterizing the geometry and dynamics of both objects. The interaction also led to the determination of the number of daughter bubbles formed by the collapse of the mother bubble.

#### *Acknowledgements*

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# **Influence of Material Properties and Mixing Dynamics on Heat Transport in Granular Materials**

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

Heat transfer in granular materials is a critical aspect of various industrial processes, from multiphase reactors to kilns and calciners. The study of heat transport in granular materials has seen significant advances in both experimental and computational domains. Discrete element method (DEM)-based simulation, a promising alternative to physical measurements, has been at the forefront of these advances<sup>1</sup>.

The DEM can be used to simulate granular flow by solving force and heat energy balances for individual particles. Heat is transferred to the particles by conduction through solid phases by particle-particle or particle-wall contacts, by conduction in a gas phase, by convection of a gas, and by radiative heat transfer in high-temperature systems. In cases where conduction in a gas phase and convection are negligible, and the temperature of the system is too low for significant radiation to occur, we consider only conduction in the solid phase as the primary heat transfer mechanism. Heat transfer by conduction occurs when two particles, or a particle and a wall, come into contact. Direct conduction between two particles depends on the collision dynamics, specifically the size of the contact area and the contact time<sup>2</sup>. Both of these parameters depend on the material properties, particularly Young's modulus, and on the rotational frequency of the stirrer.

This research focuses on investigating the heat transfer in granular materials within a vertical cylindrical agitator mixer equipped with two opposing flat blades at a 45-degree rake angle using DEM simulations. In many industrial applications, these mixers are often paired with heating jackets, which are critical for heating the granular bed to induce chemical reactions or evaporate moisture. This study evaluates the effect of rotational speed on heat transfer and analyzes particle motion at different stirrer rotational frequencies to understand how primary and secondary flows affect heat transfer efficiency. It also examines the effect of Young's modulus on heat transfer at different agitator operating speeds. Key simulation parameters and their influence

on heat transfer efficiency are detailed to improve the reproducibility and applicability of the results. Preliminary results suggest that both agitator speed and mechanical properties significantly influence the heat transfer process, highlighting potential optimizations for industrial mixing applications.

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# The Influence of Geometric Parameters of 3D Printed Structured Beds on Hydrodynamic Characteristics of Trickle-Bed Reactor

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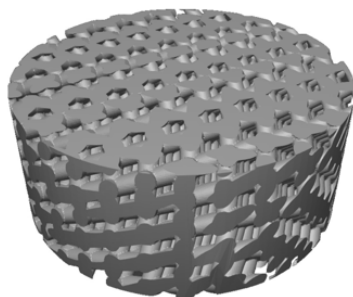
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*Supervisor: Ing. Petr Stavárek, PhD.*

*Supervising Expert: Doc. Ing. Jaromír Havlica, PhD.*

Current 3D printing methods facilitate ample opportunities for enhancing chemical reactors and their components in ways that conventional manufacturing methods cannot provide. This research aims to examine the geometric parameters of Periodic Open Cellular Structures (POCS), to assess their suitability as beds for trickle-bed reactors<sup>1,2</sup>. The study examines a parametric set of POCS structures, where cubic cell is the basic element. The parameters such as strut diameter  $sd$  and cell size  $cs$  were varied<sup>1</sup>. These modifications are implemented with an emphasis on maintaining similar porosity and specific surface area for these structures.

POCS structures were manufactured utilizing Fused Deposition Modelling (FDM) 3D printing technology with PLA material, as well



**Figure 1:** Investigated cubic POCS structure where parameters  $sd$  and  $cs$  are varied.

as Stereolithography (SLA) 3D printing method with resin material. Additionally, the study examines three types of randomly packed beds composed of spheres and two types of cylinders. Pressure drop measurements are performed in a laboratory scale under single-phase flow conditions with gas-air flow and encompass gas flow rates from 0 to 2500 dm<sup>3</sup>.h<sup>-1</sup>. The column is designed for co-current flow, with an internal column diameter of 25 mm and a height of packing of 410 mm.

In the case of POCS structures, a significant reduction in pressure drop was observed in comparison with randomly packed beds. A part of the experimental data is supplemented with data obtained by Computational Fluid Dynamics (CFD)<sup>3</sup>.

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# Bubble Breakup in Triton Solutions

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*Supervising Expert: Ing. Jaroslav Tihon, CSc.*

Hydrodynamics of bubbly flows is a broad topic, involving many interesting mechanisms and the understanding of them could help to refine chemical industry. One sub-topic that is still not fully understood is the bubble breakup<sup>1</sup> and the effect of surfactant presence on the bubble deformation before the breakup. Although it has been already shown that the presence of surfactant generally reduce the breakup frequency<sup>2</sup>, it has not yet been investigated whether surfactants only affect the surface tension or if they also affect the bubble breakup in other ways. Therefore, this work deals with investigation of the bubble breakup in surfactant Triton X-45 solutions and the results are compared with data measured in water and  $\alpha$ -terpineol solutions as another type of surfactants.

In experiments, air bubbles with equivalent diameter  $D_b$  ranging from 1.0 to 2.7 mm were interacting with vortex structures of

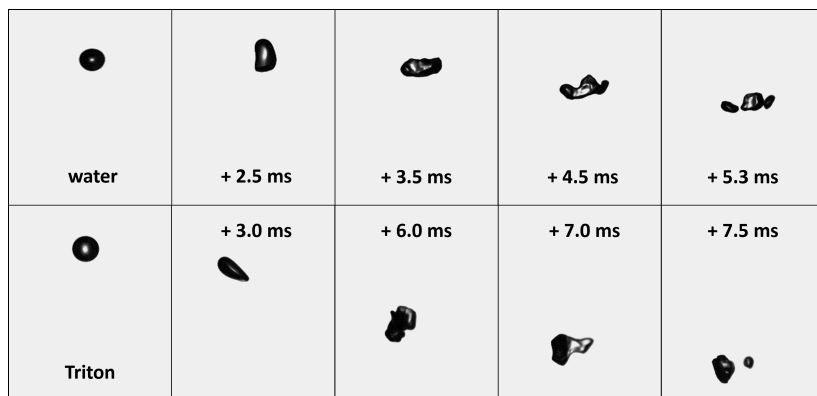


Figure 1: Example of different bubble breakup dynamic in water and Triton X-45 solution ( $22 \text{ mmol/m}^3$ ) at the same hydrodynamic conditions ( $D_b = 1 \text{ mm}$ ).

specific kinetic energy ranging from 0.27 to 2.8 kJ/kg. Interactions have been studied in two solutions of Triton X-45 with concentrations (i) 22 mmol/m<sup>3</sup> ( $\sigma = 41.8$  mN/m) and (ii) 261 mmol/m<sup>3</sup> ( $\sigma = 27.9$  mN/m). Bubble deformation and possible breakup were captured by high-speed camera and data of breakup probability, breakup time and mean number of daughter bubbles were obtained by image processing.

It was observed that the bubble breakup in presence of surfactant can be correlated by the damping time of the bubble shape oscillations. Moreover, the dynamic surface tension at actual surface age should be assumed instead of static surface tension measured in equilibrium.

#### *Acknowledgements*

The research is supported by the Czech Science Foundation through project 22-29605S.

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# Thin Film Photocatalysts on the Basis of g-C<sub>3</sub>N<sub>4</sub>

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Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) stands out as a significant metal-free photocatalyst, garnering considerable attention due to its advantageous physical, chemical, and electronic attributes. Its versatility spans across applications in photo and electrocatalysis, pollutant decomposition, water splitting, heterogeneous catalysis, and other various areas. Noteworthy is g-C<sub>3</sub>N<sub>4</sub>'s narrower band gap (2.7 eV) in comparison to TiO<sub>2</sub> (3.2 eV), indicating promising potential for light absorption, especially within the visible solar spectrum<sup>1</sup>.

This study revolves around the synthesis of powder g-C<sub>3</sub>N<sub>4</sub>, fabrication of thin g-C<sub>3</sub>N<sub>4</sub> films and their efficacy in degrading pollutants, assessed through experimentation in a batch photoreactor (BPR) and a slit geometry photomicroreactor (PMR)<sup>2</sup>. The photocatalytic activity of g-C<sub>3</sub>N<sub>4</sub> was tested with 4 different model substances: fluorescent dye, rhodamine B, was used as a reference substance and three separate antibiotics, which are emerging wastewater pollutants, namely tetracycline, trimethoprim, sulfamethoxazole<sup>3</sup>.

It was ensured that for the both reactors, the irradiating conditions were consistent by having the same frontal irradiated area, same distance from the light source, same initial concentration of a studied pollutant and all other relevant test conditions identical. The HPLC-MS method was employed to analyse the degradation products, aiding in the elucidation of potential degradation pathways. The results of photodegradation in BPR and PMR were compared via specific initial reaction rate  $r_0$  evaluated by the formula below, where  $k$  is the kinetic constant,  $c_0$  pollutant initial concentration and  $m_{\text{cat}}$  mass of the used catalyst in the reaction volume.

$$r_0 = \frac{k \times c_0}{m_{\text{cat}}}$$

The initial reaction rates were always higher in PMR in comparison to BPR. The highest specific initial reaction rate was achieved during

the photodegradation of tetracycline followed by trimethoprim, rhodamine B and sulfamethoxazole.

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Thanks to Czech Science Foundation for financial support under grant no. 23-06843S

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# Measurements of New Particle Formation in the Atmosphere

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Aerosol particles are ubiquitous in the Earth's atmosphere and they have significant impact on human health, on Earth's climatic system or on radiative forcing. Aerosol particles are emitted to the atmosphere directly from a known source, or they are formed from gaseous precursors. Molecules form clusters, which can grow into larger sizes and eventually form new aerosol particles. The cluster concentration varies during the day. Clusters start to form in the morning and then they either continue to grow or they disappear. The processes driving the aerosol formation are not yet fully understood. If the particles continue to grow, the situation is called New Particle Formation event (NPF). Besides the cluster concentration, NPF events are affected by parameters of the environment.<sup>1,2,3,4</sup>

In this work, the formation of particles and their transformation to larger sizes will be studied by measuring the concentration of molecular clusters. The measurement will take place at a rural background site National Atmospheric Observatory Košetice. At the ground level, a Neutral and Air Ion Spectrometer (NAIS) able to measure both neutral and charged clusters or particles ranging from 0.8 to 40 nm in diameter will be used together with a Particle Size Magnifier (PSM) able to measure neutral clusters as small as 1 nm in diameter up to 12 nm. Larger particles will be measured by a Scanning Mobility Particle Sizer (SMPS). At a height of 230 m above ground level, there will be another SMPS and also a nanoSMPS able to detect particles as small as 1 nm in diameter.

This combination of measuring devices allows for the coverage of continuous particle size distribution from the smallest stable clusters up to 800 nm. Additionally, this will allow the comparison of the data from ground level to that from a height of 230 m above ground level.

### *Acknowledgements*

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