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  The section is organized by ČTP SUSCHEM CZ as part of the "Suschem V" project, project registration number CZ.01.01.01/07/24_052/0005274, with the support of the Ministry of Industry and Trade of the Czech Republic and co-financing from the European Union under the OP TAK.
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PLENARY LECTURES

Profitable Solutions for Conversion of Crude to Chemicals – Lummus Technology

R. Theunissen

Lummus Technology, The Hague, The Netherlands

Refiners enjoyed strong post-Covid margins, but today's market is defined by supply-chain disruptions, volatile energy prices, and polymer oversupply, pressuring especially European assets. As smaller, less complex refineries shut down, long-term competitiveness increasingly depends on shifting more barrels crude oil to chemicals, where demand and pricing remain structurally more resilient.

Lummus Technology offers practical, high-impact pathways to accelerate this transition. Our **TC2C™ process** converts **70–85% of crude or condensate into high-value chemicals**, with the first commercial unit starting up in 2027. Key TC2C™ features can be retrofitted into many European sites to boost chemicals yield at **minimal CAPEX, OPEX and CO_2 footprint**, for example by diverting lighter crude fractions into TC2C™ conditioning to feed existing steam crackers or aromatics units.

This presentation outlines how **targeted, intelligent integration,** rather than mega greenfield projects, can immediately improve margins, expand feedstock and product flexibility, and make European refinery-petchem complexes future-proof against growing global competition.

OIL, COAL, NATURAL GAS, ALTERNATIVE RAW MATERIALS

LECTURES

CURRENT ACTIVITIES OF CTP SUSCHEM

M. Šilhan
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ČTP Suschem is working on the Suschem V project, within which it has developed an Action Plan for Digital and Green Transformation. This document contains
specific measures that are relevant for companies operating in the chemical industry.
The Action Plan is focused primarily on small and medium-sized enterprises and aims to help these companies achieve the goals of digital and green transformation. The Action Plan also includes a definition of the conditions necessary to meet the goals of digital and green transformation in the Czech Republic, both at the legislative level and in the area of support for selected new technologies and new skills.

IMPROVING COLD FLOW PROPERTIES OF BIODIESEL: EFFECTS OF FEEDSTOCK COMPOSITION, AMIDES, AND BLENDING STRATEGIES

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The work is focused on the low-temperature properties, such as cloud point (CP) and cold filter plugging point (CFPP), of methyl esters (biodiesel) produced from various types of oils and fats with different profiles of higher fatty acids (FA), such as Camelina sativa, linseed, sunflower, rapeseed, animal fats, coconut, palm kernel, and shea butter. For each methyl ester, the FA profile, iodine value, CP, CFPP, crystallization behavior determined by microscopy under different conditions (especially different cooling temperatures and ester layers), and differential scanning calorimetry were determined and compared. Biodiesel from animal fats contains more than 50% saturated fatty acids, which worsens low-temperature properties.

Moreover, the influence of amides, which were found in methyl esters from animal fats, was studied because they rapidly deteriorate low-temperature properties. The amides are present in fats and are transferred into esters during processing. They were determined by several methods, such as infrared spectroscopy and GC–MS, which enabled successful identification of fatty acid amides of palmitic, stearic, and oleic acids. Their content was correlated with low-temperature properties. Several methods for decreasing their content were suggested to remove or reduce them, thereby improving the low-temperature properties of biodiesel. Amides have higher boiling points than esters, so removal by distillation is possible but expensive. The results show that filtration and decantation can partially remove saturated fatty acid amides, which leads to a decrease (improvement) in the cloud point and CFPP.

Attention was also focused on blending fossil diesel with biodiesel from rapeseed oil and animal fats in different ratios and with different depressants influencing CFPP.

Acknowledgements
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SUSTAINABLE PRODUCTION OF ADVANCED BIOFUELS VIA CO-PROCESSING OF SELECTED NON-FOOD FEEDSTOCKS WITH ATMOSPHERIC GAS OIL

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This paper comprehensively analyses selected non-edible feedstocks in a co-process to produce advanced biofuels. The research aimed to study the co-processing of standard refinery gasoil by adding vegetable oils (camelina, karanja, mustard, post-fermentation corn oil, spent coffee ground oil) and UCO. Their effects on the activity of the $NiMoP/Al_2O_3$ catalyst and product properties in a stacked bed were evaluated. The co-process was operated at a hydrogen pressure of 5MPa, LHSV=0.7 h^{-1}, a hydrogen to feedstock ratio of 350 to 450 NL/L.h, and adding 2, 5 and 10 % by volume of different bio-oils.

Much attention has been paid to the pretreatment of feedstocks, as they have significant potential to cause catalyst deactivation. Prior to the co-processing, it was necessary to remove unwanted phospholipids and reduce the content of metal cations present in the oil. Degumming was done with citric acid at 50 °C. The washed, degummed oil was dried and refined on a silica gel column.

Within the co-process's measured pressure and temperature range, complete deoxygenation of free fatty acids and glycerides to alkanes (acid number and simdist) occurred. The cracking rate was minimal. The C_{5+} yield was above 97,5 %.

The distribution of n-alkanes in the product shows that the proportion of C_{15}-C_{19} n-alkanes increased, resulting in a marked increase in the cetane index from 54.1 to 59.6-62.2. The low-temperature properties met the normalised values for the summer season when 2, 5, and 10 % by volume of bio-oils were injected. The aromatic content was significantly reduced, especially di- and polyaromatics.

At 360 °C, 50 bar H_2 pressure, an LHSV of 0.7 h^{-1}, and a hydrogen-to-feedstock ratio of 250 NL/L, a sulphur content limit of 10 mg/kg was achieved only in the case of at 2 and 5 % vol. PFCO addition. Under the same conditions, adding 2, 5, and 10 % vol. of other tested bio-oils did not achieve the 10 mg/kg sulphur content limit, and the hydrogen-to-feed ratio had to be increased. During co-processing, triacylglycerides were completely converted to hydrocarbons. The increased content of unsaturated bonds in bio-oils also negatively affected compliance with the sulphur content limit in co-processed products.

Conversely, adding 2-10 % by volume of bio-oil had no significant adverse effect on the low-temperature properties of the products. Pretreatment of bio-oils is a prerequisite for their use in co-processing

Keywords
post-fermentation corn oil; advanced biofuels; hydrodeoxygenation; catalyst; co-processing
Acknowledgements
The Slovak Research and Development Agency has financially supported this research under contracts APVV-18-0348, APVV-18-0255 and APVV-20-0348.

ANALYSIS OF SUSTAINABLE AVIATION FUELS AND PREDICTION OF HEFA CONTENT USING ATR-FTIR AND GC×GC-MS/FID

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At present, one of the most important strategies for reducing greenhouse gas emissions is the implementation of alternative aviation fuels. Both passenger and cargo air transport contribute substantially to total transportation-related greenhouse gas emissions. By its nature, aviation is a global industry; therefore, mitigation efforts are coordinated by international organizations. At the European level, a legislative framework has already been established, for example Regulation (EU) 2023/2405, known as ReFuelEU Aviation. This regulation defines the minimum required share of sustainable aviation fuels depending on the target year. These requirements also raise the question of whether compliance can be reliably monitored and verified. Fossil-based and alternative aviation fuels generally exhibit very similar hydrocarbon structures, which makes their quantification in blended fuels analytically challenging. Currently, the only reliable method is radiocarbon (^{14}C) analysis, which is relatively demanding in terms of time and cost.

This work focuses on the development of alternative analytical approaches employing ATR-FTIR spectroscopy, comprehensive two-dimensional gas chromatography coupled with mass spectrometry and flame ionization detection (GC×GC-MS/FID), and multivariate statistical analysis. The fuels investigated include Jet A-1, HEFA, AtJ, CHJ, and SIP. For blends of HEFA and Jet A-1, predictive models for determining HEFA content were developed, achieving a root mean square error of prediction (RMSEP) below one percent by volume.

FROM CLASSICAL TITRATION TO A SMART LABORATORY: AUTOMATED DETERMINATION OF TAN AND TBN ON THE OMNIS PLATFORM

P. Majzlík, P. Barath
Metrohm Česká Republika, s.r.o., Na Harfě 935/5c, Praha

The determination of the total acid number (TAN) and total base number (TBN) ranks among the essential analytical techniques for evaluating the technical condition of oils and lubricants. In today's industrial environment, however, these established methods are increasingly becoming part of fully digitalized and automated laboratory ecosystems aligned with Industry 4.0 principles.
This contribution introduces a fully automated solution for TAN and TBN analysis built on the modular Metrohm OMNIS platform. OMNIS enables seamless automation of the entire workflow—from sample preparation, solvent and reagent dispensing, and electrode cleaning to the titration process, digital data evaluation, and secure archiving. This high level of automation minimizes operator influence, enhances reproducibility, and allows continuous operation while ensuring full compliance with relevant ASTM and ISO standards.
The digital architecture of the OMNIS platform further supports complete data traceability, advanced statistical evaluation, and effortless integration with LIMS or enterprise-level databases. As a result, TAN and TBN determinations evolve from traditional standalone laboratory analyses into strategic tools for predictive maintenance, quality assurance, and overall operational cost optimization.
This contribution demonstrates how classical titration techniques can be efficiently transformed into smart, future-ready laboratory technologies that fully meet the demands of modern digital industry.

HIGH-RESOLUTION MASS SPECTROMETRY FOR THE CHARACTERIZATION OF COMPLEX OXYGENATED MIXTURES

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High-resolution mass spectrometry (HRMS) represents a powerful analytical approach for the characterization of complex mixtures, providing partial structural information on compounds that are not accessible by conventional GC-MS analysis. To better understand the influence of ionization mode on the detection of oxygen-containing compounds, a set of model substances representing major oxygenated classes, including phenols, furans, dimethoxyphenols, carboxylic acids, and carbohydrates, was selected. In addition, four pyrolysis oils derived from the pyrolysis of cellulose, hemicellulose, and lignin from both softwood and hardwood were analyzed, representing the principal structural components of biomass. The samples were analyzed using several HRMS ionization techniques, such as atmospheric pressure chemical ionization (APCI), electrospray ionization (ESI), and soft

ionization by chemical reaction in transfer (SICRIT) ionization, each operated in both positive and negative modes. Comparison of the responses obtained for the model compounds and for the pyrolysis oils allows evaluation of which ionization methods provide the most comprehensive and representative characterization of their molecular composition.

THE PRESENCE AND FUTURE OF STEAM CRACKING IN EUROPE

J. Doskočil
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The petrochemical production in Europe is facing a significant pressure from different areas – the regulatory, market, geopolitical and even process design constraints have impact on this industry and its profitability. From the regulation point of view the EU policy of the decarbonization, implementation of green electricity and plastic waste recycling are broadly promoted as the tools paving the way to circular economy. Despite the fact there is no doubt the final task is reasonable and legitimate the way how to achieved it in industrial scale is very uncertain and poorly defined. Moreover, the impact of EU Council regulations is permanently increased by the introducing of the more strict goals and complicated by the profit extraction via different penalties and emissions allowances.
Such a kind of regulatory obstacles complicates the possibility to keep the plants running profitably at European Union. All companies indicate energy cost competitiveness in Europe as the primary rationale for assets closing – and majority of them also notes that demand-related considerations, overcapacity and regulatory factors are the additional issues.
The uncompetitive energy cost in Europe is logically triggering the pressure on the finding of an effective solution of this problem. As always, in case there is a cheaper source of product and the logistics costs are not making and obstacle, the unprotected market can be flooded by imported goods – especially when the guarantied quality is the same like in case of polymers. The huge capacities installed in the Middle East countries are the source of polymers imported to Europe – as fast as the import grows the European capacities are closed with the same pace. Nevertheless the problem of extreme energy costs can be solved in different way too – by the implementation of the new more effective, less energy demanding and more environment friendly technologies. However, such an approach is a basic feature of decarbonisation. Despite that, the overall investment in petrochemical segment in Europe were decreased five times during the period of last three years.
The importance of geopolitical factor becomes extremely critical during last few months as can be seen from TV news every day. The combination of the war conflicts at Ukraine and the Middle East with the planned abandonment of natural gas supplies from Russia (2027) raise oil and natural gas prices to a level comparable to that achieved during year 2022. However, the overall geopolitical situation is much more worse and less predictable – this fact complicates significantly financing and justification of the principal CAPEX projects. Simply, the important decisions related to the big investment projects about the

raw materials sources, feed stocks composition, energy sources, etc. cannot be made in a way that design driving parameters are changed very soon after commissioning or even during construction phase.
Last but not least, the implementation of decarbonization projects can be complicated or limited by existing plant configuration. Although the decarbonization is a feasible approach it is clear its potential can be very different based on multiple parameters (e.g. design of the plant, year of commissioning, cracked feed stock and many others). The implementation of decarbonization projects needs complex analysis of the plant configuration and operation and it can trigger further investments that would be necessary for successful completion of the project.
The situation of the petrochemical industry in Europe is alarming. The pressure on the implementation of decarbonization projects in combination with other mentioned threats leads to the situation when the closure of assets in Europe is economically more advantageous than keeping the plants running in totally uncompetitive environment. The existing technical solutions are able to solve a lot of decarbonisation and recycling related problems but without the provision of the equal business chances will be European petrochemical industry probably doomed to extinction.

MATERIÁLOVÁ BILANCE KOKSU JAKO NÁSTROJ HODNOCENÍ DOPADU VÝPADKU ELEKTŘINY NA PROVOZ PYROLÝZNÍCH PECÍ ETYLENOVÉ JEDNOTKY

P. Vitiska, P. Michalička, O. Ottenschläger
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Výpadek dodávky elektřiny v České republice v roce 2025 představoval mimořádnou provozní událost s přímým dopadem na kontinuální technologické celky petrochemického průmyslu. Předkládaný příspěvek analyzuje vliv této události na pyrolýzní sekci ethylenové jednotky společnosti ORLEN Unipetrol v Litvínově, se zaměřením na dynamiku odstavení a následné řešení provozních problémů pyrolýzních pecí.
Text systematicky popisuje průběh náhlé ztráty napájení, odezvu technologických uzlů (hořákové systémy, přívod suroviny, parní ředění, tah spalin) a přechod jednotky do havarijního režimu. Zvláštní pozornost je věnována změnám teplot ního a tlakového profilu vlásenek, dočasné ztrátě optimalizovaného poměru uhlovodík/pára a jejich vlivu na nežádoucí reakce vedoucí k intenzifikaci koksotvorných mechanismů (radikálová polymerace, kondenzace aromátů, katalytická depozice na kovovém povrchu).
Na základě množství koksu odstraněného při sanačních zásazích je zpětně kvantifikována intenzita koksotvorby v dotčeném provozním cyklu pyrolýzní pece. Analýza vychází z dat získaných během následného odstranění koksu, přičemž část pecí byla úspěšně regenerována standardní oxidační metodou, zatímco u některých pecí došlo k tak výrazné depozici koksu ve vlásenkách, že nebylo možné obnovit jejich průchodnost běžným postupem a bylo nutné přistoupit k mechanickému čištění.
V textu jsou hodnoty následně porovnány s referenčními bilancemi koksu experimentálně stanovenými periodickým odběrem spalin (CO/CO_2) s následnou hmotnostní bilancí

oxidovaného uhlíku během standardních provozních cyklů. Porovnání umožňuje objektivně vyhodnotit rozsah a závažnost dopadu mimořádné události na koksotvornou dynamiku pyrolýzní sekce.

EXPERIENCE IN THE DESIGN AND CONSTRUCTION OF CHEMICAL PROCESS UNITS

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During both the design and construction phases of a chemical process unit, various technical challenges may arise. Many of these issues are related to mass transfer in reactors and distillation columns. Another common challenge involves off-gas handling systems, particularly their disposal capacity. The availability of utilities, such as cooling water and steam, is also a critical factor in the successful operation of the process unit.
This presentation will provide examples of the above-mentioned challenges and share practical experience on how these issues were addressed.

MODEL BASED OPTIMIZATION OF DISTRICT HEATING NETWORK OPERATION

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District heating systems play a crucial role in improving energy efficiency and reducing environmental impacts in urban areas. This paper presents the design and analysis of a dynamic control strategy for a model district heating network, with a focus on improving both energetic and economic performance. A quasidynamic mathematical model of the heating network was developed, combining a steady state hydraulic model for mass flow distribution with a dynamic thermal model describing unsteady temperature propagation in the pipeline system. The model was implemented in the MATLAB environment.
Pressure losses, heat losses, and transient operating states were analyzed to capture realistic network behavior during load changes. Two control strategies were investigated and compared: control based solely on mass flow variation and combined control using both mass flow rate and supply temperature. An optimization framework was employed to minimize operational costs while ensuring full coverage of heat demand.
In addition, the impact of integrating a cogeneration unit into the system was evaluated. The results demonstrate that combined temperature and flow control provides superior performance compared to flow-only control, leading to reduced operating costs and improved system efficiency.

This study was supported by the Slovak Research and Development Agency under contract no. APVV-18-0134 and APVV-19-0170. The authors acknowledge the financial support from the Slovak Society of Chemical Engineering.

VLIV PŘÍDAVKU PYROLYZÁTU NA VÝTĚŽKY PYROLÝZY PRIMÁRNÍHO BENZINU

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Tato práce se zabývá analýzou pyrolýzy primárního benzinu ve směsích s pyrolýzním olejem z odpadních plastů. Za cíl si klade vyhodnotit vliv alternativní vstupní suroviny na výtěžky klíčových produktů. Různé směsné poměry byly použity pro posouzení výtěžků pyrolýzy prováděné za stejných provozních parametrů. Výsledky byly porovnány s výtěžkovými vektory pyrolýzy běžného primárního benzinu a primárního benzinu ve směsi s pyrolýzním benzinem.

Rozdílné složení vstupní suroviny a příslušné výtěžkové vektory společně naznačují trendy při případném začlenění alternativních surovin do surovinové základny petrochemických procesů. Klíčovým parametrem se jeví obsah nenasycených a aromatických sloučenin ve vstupní surovině, jelikož úzce souvisí s průběhem nežádoucích vedlejších reakcí (tvorba vysokomolekulárních látek).

Práce rozšiřuje znalost chování alternativních surovin v procesu pyrolýzy a naznačuje limity a možná úskalí „udržitelných“ produktů. Diskutovány jsou rovněž provozní strategie a technologické úpravy, které mohou podpořit průmyslové využití směsných surovin v pyrolýze.

FULL-SCALE EXPERIMENTS AT STEAM CRACKER UNIT

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The process of crude oil processing and the production of petrochemicals with the arrival of new legislative requirements for sustainability and sustainable development requires a change in the commonly used feedstocks. Within the European Union, there are several initiatives for research and innovations that focus on replacing fossil fuels with alternative feedstocks. As part of decarbonization and the circular economy, Orlen Unipetrol has become a member of the Horizon Europe program with its Clear Up project.

The transition to a different type of feedstock means that it will be necessary to perform a lot of full-scale experiments. In order for full-scale testing to be possible, two main

challenges need to be solved: mechanical set-up and sufficient amount of alternative feedstock.

There is currently not enough alternative feedstock on the market, as the production of pyrolysis oil from plastic waste is still being optimized to ensure that the quality of the oil is reproducible and meets the quality parameters for further processing. For this reason, it was decided to use recycled pyrolysis gasoline as a model feedstock for our purposes. Pyrolysis oil from waste plastics has a similar composition to recycled pyrolysis gasoline, which provides valuable insights for future integration of alternative feedstock into the steam cracking process. Several tests have been carried out so far, in which pyrolysis gasoline was blended with primary gasoline in order to determine basic technological findings such as the retention time of the pyrolysis gasoline in the pipeline.

Within the mechanical settings, a smooth and continuous supply of recycled pyrolysis gasoline must be ensured. This requires the construction of a pipeline connection between the pyrolysis gasoline hydrogenation unit and the DCPD production unit with a primary gasoline feedstock tank. In addition to the pipeline connection, this set-up also requires the installation of a pump and a certified flow meter.

PYROLYSIS OF TETRAPAK

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Plastic recycling represents a current challenge in materials and environmental research, with growing interest in the efficient management of multi-layer packaging such as Tetrapak-type beverage cartons. Tetrapak is a multi-layer packaging material used for packing beverages and food. It consists of approximately 75% paper, 20% polyethylene, and 5% aluminum foil.
In industrial practice, mechanical recycling currently dominates, producing secondary materials such as construction boards. A more advanced recovery approach is represented by the technology of Plastigram Industries a.s., which is based on defibering the cellulose layer for paper recycling. The remaining polyethylene–aluminum fraction is then mainly processed by material recycling, resulting in lower-quality products used primarily in construction applications. A more promising alternative is chemical recycling, which enables effective separation of plastic from aluminum and their subsequent chemical reuse without significant loss of quality. Among chemical recycling methods, pyrolysis is considered one of the most effective. It is a thermal decomposition process carried out in an inert atmosphere, producing oil, gas, and solid residue. A key advantage of pyrolysis is its ability to treat mixed or contaminated materials, which are essential for multi-layer packaging. In the case of Tetrapak, pyrolysis allows aluminum to remain mainly in the solid product, while most of the plastic is converted into hydrocarbon-rich pyrolysis oil. Process

optimization is necessary to maximize product yields and improve oil quality. This research aims to evaluate the effect of reaction conditions on the yields, composition, and properties of products obtained from Tetrapak pyrolysis.
The objective is to obtain pyrolysis oil with the lowest possible final boiling point to enhance its suitability for steam cracking and monomer production.
This presentation will summarize the boiling range adjustment and the detailed analysis of group composition and key contaminants, particularly oxygenates and aluminum.

Acknowledgment
The work was supported from the state budget of the Technology Agency of the Czech Republic under the program SIGMA DC2 (project TQ15000068).

UPGRADING OF PLASTIC PYROLYSIS OIL TO STEAM CRACKING FEEDSTOCK

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The chemical recycling of waste plastics via pyrolysis offers a promising route toward circular production of petrochemicals. Pyrolysis oils derived from mixed plastic waste can, in principle, serve as alternative feedstocks for steam cracking. In practice, however, their direct utilization is limited by an extremely broad boiling range and, particularly, by heteroatom concentrations exceeding conventional steam cracker specifications. Targeted upgrading is therefore essential to unlock their full potential.

In this contribution, we present an integrated hydroprocessing strategy for upgrading the oil produced by continuous industrial pyrolysis of mixed post-consumer polyolefins. The oil was waxy at room temperature with a boiling range extending beyond 600 °C and contained significant levels of nitrogen and trace metals. Hydroprocessing was conducted in a continuous, fixed-bed reactor over a wide operating window to identify optimal upgrading pathways.

The process consisted of two consecutive catalytic steps. First, hydrotreatment over a sulfided Ni–Mo/γ-Al_2O_3 catalyst effectively reduced nitrogen content to below 25 mg/kg, protecting the hydrocracking catalyst from deactivation. This was followed by hydrocracking over a sulfided Ni–W catalyst, with reaction conditions tuned to maximize boiling-range reduction and tailor product composition. Two alternative pathways were evaluated: hydrocracking of the full pyrolysis oil and hydrocracking after prior removal of the naphtha fraction.

The presentation will highlight:
- The effect of hydrotreatment temperature on olefin saturation and heteroatom removal.
- The influence of hydrocracking conditions on final boiling point reduction and product quality with respect to steam cracker feed requirements.
- The potential benefits of naphtha cut removal, including hydrogen savings.
- A comparative assessment of both hydroprocessing routes, supported by an overall mass balance from plastic waste to steam cracker feedstock.

STEPS TOWARD SUSTAINABILITY IN PETROCHEMICAL PRODUCTION: FOCUSING ON RENEWABLE BIO-ALCOHOLS

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Petrochemical plants producing key chemicals such as ethylene, propylene, aromatics and other chemicals for the production of everyday products are experiencing difficult times, especially in Europe. These are highly energy-intensive processes in which hydrocarbon raw materials (ethane, middle distillates, HCVD) are thermally cracked into the above-mentioned chemicals. In addition to energy prices, the segment is burdened by oil prices, transport fees, and also emission allowances and labor costs. Last but not least, there is the inherent influence of the raw material, in which the yield of the key ethylene decreases with increasing length of the hydrocarbon chain in the raw material. From this point of view, central European ethylene units are no longer competitive. Ethylene and propylene form the basis for important chemical products of everyday life from plastics (PP, PE), farmaceutical drugs, textiles, etc. In Europe, 18-20 million tons of ethylene and 14-15 million tons of propylene are produced in 48 units. Unfortunately, there is an actual risk of closure of up to 40% of the manufacturing plants.
Despite the unfavorable situation, "green" solutions defined in the Green Deal continue to be legislatively promoted. However, the present-day scarcity of sustainable raw materials (e.g., pyrolysis oil, ethanol) hinders the comprehensive replacement of ethylene and propylene production Nevertheless, petrochemical products that are used in subsequent technologies, such as copolymers of polymerization (hexene, butene), can be gradually replaced. These can be prepared from ethylene by oligomerization or dehydration of the relevant alcohols. Our work is focused on the preparation of higher alcohols from ethanol usable for the production of olefins with use in petrochemicals in the production of polyethylene and polypropylene.

Acknowledgement
This research is co-financed from the state budget by the Technology agency of the Czech Republic under the National Centres of Competence Progamme TN02000044.

SELECTIVE DEHYDROGENATION OF BIOETHANOL ON CU/LIAL MIXED OXIDES

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The work deals with the catalytic conversion of bioethanol on Cu-modified LiAl mixed oxides. Bioethanol is an important platform molecule obtained by fermentation of biomass, and its further transformation offers a path to sustainable chemical intermediates. One potential option is its conversion to higher alcohols via the Guerbet reaction, but selective control of individual reaction steps remains a challenge.
A series of LiAl mixed oxides with different Li/Al molar ratios (0.2–5) was prepared, which were characterized by different acid-base, textural properties, and phase composition. Copper (0.6–10 wt.%) was then incorporated into these materials using an impregnation method involving melamine, which contributed to the stabilization and dispersion of Cu particles. Detailed physicochemical characterization showed that the combination of the Li/Al ratio and copper content significantly affects the dispersion of copper and the surface properties of the catalysts.
Catalytic tests conducted at 200 to 400 °C under atmospheric pressure showed that the dominant reaction is the dehydrogenation of bioethanol to acetaldehyde. The conversion of bioethanol reached approximately 45% (at a loading of 4.5 h^{-1}) and the selectivity to acetaldehyde was very high (98–99%), while the formation of higher alcohols was negligible. The results suggest that the dehydrogenation step proceeds very efficiently, but the subsequent steps of the Guerbet reaction (aldol condensation, dehydration, and hydrogenation) are significantly limited under the given conditions. The study contributes to a deeper understanding of the relationship between the composition, structure, and catalytic behavior of Cu/LiAl systems in bioethanol conversion.

Acknowledgements
This work was supported by the Internal Grant Agency of the University of Pardubice, Czech Republic (SG_36_2006).

CHEMICKÁ RECYKLACE JAKO ALTERNATIVNÍ ZDROJ SUROVIN PRO PETROCHEMII.

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Termochemické metody chemické recyklace plastů – pyrolýza a gasifikace – představují hlavní alternativní zdroj surovin nejen pro petrochemický průmysl a podporují cirkulární ekonomiku. Globální produkce plastů dosahuje kolem 460–470 milionů tun ročně (2024–2025), přičemž recyklace zůstává nízká (9–15 %). Termochemické procesy umožňují zpracování směsných a kontaminovaných odpadů.

Pyrolýza produkuje pyrolýzní olej, upravitelný na vstupní surovina pro parní krakování (výroba olefinů) nebo jej lze katalyticky upravit na směs aromátů označovanou jako BTX (benzen, toluen, xyleny) s výtěžností až 17–40 %, Ty pak nahrazují aromáty z černouhelného dehtu pro plasty (PS, PET), barviva a rozpouštědla. Gasifikace pak generuje syngas ($CO + H_2$) pro metanol, popř. olefiny (technologie MTO). Zpracovat lze ale pomocí Fischer-Tropschových reakcí na paliva nebo využít separovaný vodík na výrobu amoniaku Haber-Boschovu syntézou.

Výstupy klasifikované jako Recycled Carbon Fuels (RCF) v rámci směrnice EU RED II, resp. RED III přispívají k dekarbonizaci dopravy, v kombinaci s využitím „zeleného“ vodíku je pak lze vykázat i jako hybridní RNFB paliva, tento proces je klíčem k výrobě e-paliv. LCA ukazují úsporu GHG až 75 % oproti fosilním surovinám.

V Evropě je v provozu 18 zařízení s kapacitou 289 kt/rok (převážně pyrolýza 262 kt), prozatím však žádná komerční zařízení ke gasifikaci. Plánováno je nicméně 65 projektů s 2,8 Mt/rok (pyrolýza 1,94 Mt, gasifikace 0,86 Mt). Nejznámější projekty: ExxonMobil (Baytown, Texas: zdvojnásobení na 500M liber/rok); BASF ChemCycling (integrace pyrolýzního oleje, Ccycled produkty v USA/EU); Plastic Energy (druhá továrna Sevilla, Španělsko: 33 kt/rok); Neste (rozšíření Porvoo, Finsko); Eastman (Kingsport methanolýza). Odhad růstu trhu (CAGR >25 %) signalizuje přechod k udržitelné petrochemii, snižující závislost na fosilních zdrojích. Tento růst bude tažen i poptávkou po recyklovaném obsahu v obalech, kterou vyžaduje nová evropská legislativa (PPWR – Packaging and Packaging Waste Regulation).

OIL, COAL, NATURAL GAS, ALTERNATIVE RAW MATERIALS

POSTERS

HOW TO DETERMINE OLEFINS IN PYROLYSIS/HTL OILS FROM WASTE PLASTICS AND TIRES USING GC×GC-FID?

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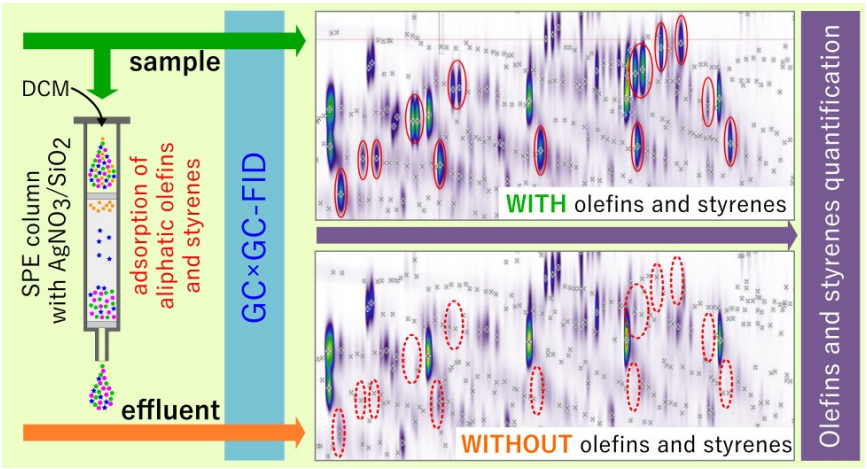
Olefins create the major hydrocarbon group in pyrolysis oils from waste plastics and tires, accounting for over 70 wt%. As olefins are responsible for low thermo-chemical stability and difficulties during the valorization of those oils, the reliable and accurate determination of olefins is thus essential.

The identification of olefins, even with high-resolution techniques such as GC×GC, remains challenging without a specific detector, like PI-TOF-MS or VUV. Currently, the only method for the selective determination of olefins in plastic pyrolysis oils is GC-VUV, which has recently been standardized as ASTM D8519. However, PI-TOF-MS and VUV are not affordable instruments for many research teams working on plastics recycling.

This poster will present a simple method recently developed and published [1] by our team. The method is based on a micro-scale adsorption of olefins over $AgNO_3/SiO_2$, followed by the GC×GC-FID analysis. Olefins are determined indirectly from the loss of chromatographic area in respective chromatogram regions before and after their removal. The method requires a small sample volume (≈50 µL) and ≈approximately 15 minutes of sample separation. The method was extensively validated and provides a reliable determination of olefin content in oils from plastics and tires, as well as their products after mild hydrotreatment. This method is affordable for all researchers and industrial companies working on plastic recycling by thermochemical processes, as it does not require an MS detector.



[1] M. Auersvald, et al. Talanta 281 (2025) 126792.
https://doi.org/10.1016/j.talanta.2024.126792.

HYDROCRACKING OF PYROLYSIS OIL FROM WASTE POLYOLEFINS

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Pyrolysis is a promising process that enables the depolymerization of waste plastics into products such as pyrolysis oil (PO), which can be further utilized to produce fuels or monomers. The valorization of PO as a feedstock for steam cracking appears to be one of the most promising routes for the chemical recycling of plastics. However, waste plastics are contaminated, which leads to an increased content of heteroatom-containing compounds in the oil. PO also contains a high proportion of olefins, both exceeding the limits required for steam cracking feedstock. Therefore, improving the quality of PO is essential for its use as a feedstock for monomer production. Promising upgrading methods include hydrotreating and hydrocracking, which were the focus of this research.
The main objective of hydrotreating was to reduce the nitrogen content (≈3100 mg/kg) and the olefin content (≈47 wt.%) in the studied PO to meet steam-cracking limits. The aim of hydrocracking was to decrease the final boiling point of PO and maximize the yield of the fraction boiling below 200 °C. The studied PO was produced from polyolefin-rich waste plastics and was solid under laboratory conditions. The study investigated hydrocracking of the whole oil after hydrotreating as well as hydrocracking of the hydrotreated fraction with a boiling point above 200 °C. The results demonstrated that hydrogenation-based upgrading is an effective route to improve the quality of PO for steam cracking.

ZMAPOVÁNÍ STAVU ETHANOVÉ PYROLÝZNÍ PECE POŠKOZENÉ BĚHEM VÝPADKU DODÁVEK ELEKTRICKÉ ENERGIE

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Dne 4. července 2025 postihly rozsáhlé a závažné výpadky dodávek elektrické energie severní Čechy, části středních a východních Čech a východní polovinu Prahy. Výpadek proudu byl způsoben pádem 400 kV elektrického vedení V411 v severních Čechách a následným odpojením elektrárny Ledvice B6 o výkonu 650 MW od sítě. Výrazný rozdíl mezi dodávkou a spotřebou elektřiny způsobil nestabilitu sítě a odpojení 9 důležitých rozvodných (spínacích) stanic.
Obě rozvodné stanice zásobující společnost ORLEN Unipetrol (Výškov a Chotějovice) patřily mezi výše uvedených 9 jednotek, zařízení Chempark v Záluží bylo postiženo výpadkem proudu přibližně ve 12:03 hodin. Výpadek elektrické energie v jednotce monomery začal ve 12:03 hodin a trval do 17:05 hodin. Způsobil nejen přerušení dodávky

elektrické energie, ale také dodávky chladicí vody, páry, dusíku, BFW a instrumentárního vzduchu.
V době výpadku elektrické energie bylo na pyrolýzní sekci Ethylenové jednotky v provozu 7 pyrolýzních pecí (4 benzín, 1 LPG, HCR a ethan). Výpadek proudu způsobil okamžité odstavení veškerého zařízení Ethylenové jednotky i navazujících jednotek. Došlo k extrémním změnám tlaku, teploty a průtoku uvnitř zařízení. Celá pyrolýzní sekce byla velmi negativně ovlivněna vypnutím všech provozovaných pyrolýzních pecí (prudký pokles teploty, smrštění vlásenek), to mělo za následek ucpání (zakoksování) pyrolýzních vlásenek, poškození trubek kotlů na odpadní teplo a závažné zničení radiace ethanové pece BA-107. Cílem bylo zmapovat zničené pyrolýzní vlásenky v peci BA-107, (vrstva koksu v jednotlivých výškových úrovních) a na příkladu jednoho z pyrolýzních reaktorů diskutovat tvorbu uhlíkatých úsad v závislosti na délce reaktoru a provozních podmínkách.

CHARACTERIZATION OF WASTE LDPE AND PP PYROLYSIS CHAR

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The solid residue produced during the thermal cracking (pyrolysis) of waste plastics is currently in the early stages of research and is mainly landfilled. It is called “waste plastic pyrolysis char, WPPC” and contains a high proportion of carbon and mineral fillers. Minor components include metals from polymer production and various residues from the conversion of antioxidants, functional additives, and surface contamination. The composition is largely influenced by feedstock, reaction temperature, and other process parameters. Information on the composition and morphological properties of the solid residue from plastic pyrolysis can be used to modify it for further applications.
Solid residues from the thermal pyrolysis of separated waste polypropylene and waste LDPE, as well as their mixtures, were tested in a continuous conical reactor using CO_2 as the carrier gas. The content of combustible components ranged from 23.4 to 34.6% by weight, depending on the reaction temperature and process parameters. The hydrocarbons on the surface of the solid residue ranged from C_{10} to C_{40}. Calorific value was 8.01 and 12 MJ/kg, with a specific surface area of 2.3 m^2/g. A detailed analysis of the solid residue is presented.

Keywords
Waste plastics pyrolysis char, carbon rich material, thermal cracking, mineral ash.

Acknowledgements
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SYNTHESIS AND PRODUCTION OF PHARMACEUTICALS

LECTURES

UNLOCKING THE SECRETS OF PHARMACEUTICAL POWDERS USING INVERSE GAS CHROMATOGRAPHY

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In pharmaceutical oral solid dosage drug delivery, we typically start with the drug substances and excipients in powder form. Powders are generally complex systems that can exhibit multiple surface energy values, which can be influenced by various factors such as crystal faces, edges, defects, impurities or physical states, all of which can alter the final surface properties. All pharmaceutical unit operations begin with initial surface contact. Furthermore, the surface properties of powders are an important factor to consider as they are crucial for understanding their behavior before formulating a drug substance into a dosage form. Moreover, it can be expected that surface interactions will influence the ease of production (such as mixing, granulation and tableting), the dissolution rate and subsequently the ultimate biological fate and the stability, all of which are affected by surface contact. For these purposes, inverse gas chromatography (IGC) is a valuable and powerful tool that can accurately and reproducibly probe the nature of powder surfaces by analyzing retention behavior. IGC is extremely well suited to the study of powders because this technique provides data that can explain how the surface of materials changes during processing, and how these changes affect behavior and performance of both drug substances and excipients.
The contribution is devoted to the significance and utility of surface energy which can allow predictions of powder behavior during processing.

ROLE OF SEEDED CRYSTALLIZATION IN PROCESS CONTROL AND MORPHOLOGICAL STABILITY

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The preparation of final API substances is typically carried out through controlled crystallization, which enables precise regulation of crystal size, shape, polymorphism, and purity. One of the most commonly employed methods for controlling the crystallization process is **seeding**, i.e., the intentional introduction of an appropriate crystalline material into a supersaturated solution to initiate heterogeneous nucleation and stabilize subsequent crystal growth. Although this technique is a long-established and widely used tool in crystallization control, practical challenges persist regarding the **optimal seeding temperature, the appropriate quantity of added seed material, and the selection of its physical properties**. These parameters significantly influence nucleation kinetics, the

resulting particle size distribution, and the overall reproducibility of the process. This study therefore focuses on a systematic evaluation of key seeding parameters and their impact on the stability and control of the crystallization process in the production of active pharmaceutical ingredients.
This work presents a study of the controlled crystallization of mycophenolate mofetil, focusing on the influence of different seeding materials on nucleation kinetics and subsequent crystal growth. The experimental campaigns were conducted using the **Blaze** laser probe, which provides continuous in-situ characterization of the system by generating real-time particle size distribution profiles and monitoring their temporal evolution. Simultaneously acquired images enable detailed observation of morphological changes throughout the crystallization process. The integration of controlled seeding with advanced PAT analytics thus allows for a comprehensive assessment of the stability, reproducibility, and dynamics of the crystallization process of this pharmaceutically relevant compound.

ITACONIC ACID DERIVATIVES: FROM POLYMERS TO IMMUNOMODULATING AND ANTIMICROBIAL AGENTS

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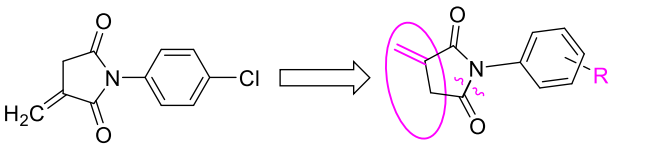
Itaconic acid (IA; methylenesuccinic acid) is an unsaturated dicarboxylic acid traditionally used as a versatile building block in polymer synthesis. IA is produced biotechnologically by *Aspergillus terreus*. Resulting polymers find applications in the food, textile, paint, and pharmaceutical industries (e.g., drug delivery systems, coatings). More recently, IA has been recognized as a mammalian endogenous immunostimulatory agent, exhibiting also multiple antimicrobial properties. Moreover, IA derivatives have been studied for antibacterial, antiviral, anticancer, antioxidant, and anti-inflammatory properties.[1,2,3]
During our search for antitubercular agents, we identified IA-based imide **1** as a broad-spectral antifungal agent at low micromolar concentrations. This finding prompted a systematic structure-activity relationship (SAR) study of IA derivatives (Fig. 1).
The amides were synthesized *via* a high-yield two-step procedure. Itaconic anhydride was reacted with substituted anilines in refluxing benzene to afford itaconic monoamides, which were subsequently converted into itaconimides by dehydrative cyclization using sodium acetate in boiling acetic anhydride.
Biological evaluation provided valuable insights into SAR. High and selective antifungal action (MIC from 3.91 μM) was observed exclusively for cyclic imides derived from IA, but not from its analogues (e.g., succinic, 2-methyl/allylsuccinic, cyclopropane-1,2-dicarboxylic, or citraconic acids), and aniline substituents such as halogens, (O)CF_3, and *tert*-butyl carboxylate, with polyhalogenation leading to improved activity.
Future work will focus on more sustainable amines (e.g., amino acids). The use of benzene represents an additional disadvantage of the synthesis of IA-based drug candidates.



initial antifungal hit **1** expanding chemical space

Fig. 1. Design of IA-based antifungal agents

This work was supported by Ministry of Health of the Czech Republic, grant nr. NW24-05-00539.

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POLYMORFIE API: VĚDA, RIZIKA A PATENTOVÁ SÍLA

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Polymorfie farmaceutických látek představuje kritický parametr ovlivňující jejich fyzikálně-chemické vlastnosti, technologické zpracování i dlouhodobou stabilitu léčivých přípravků. Různé polymorfní modifikace mohou vykazovat výrazné rozdíly v rozpustnosti, termodynamické a kinetické stabilitě či mechanickém chování, což zásadně ovlivňuje biofarmaceutický profil i robustnost výrobního procesu. Z tohoto důvodu generické společnosti rutinně provádějí rozsáhlý polymorfní screening s cílem identifikovat všechny relevantní pevné formy API, porozumět jejich transformačním vztahům a minimalizovat riziko neočekávaných konverzí během výroby nebo skladování.

Klíčovým aspektem je detailní poznání stabilitního chování jednotlivých modifikací a faktorů, které indukují jejich přeměny, včetně vlhkosti, teploty či mechanického stresu. Tyto informace umožňují navrhnout prediktivní kontrolní strategii a zajistit konzistentní kvalitu produktu během celého životního cyklu.

Polymorfie však představuje nejen vědeckou a technologickou výzvu, ale také významný strategický prvek v oblasti duševního vlastnictví. Identifikace nové polymorfní formy umožňuje vytvoření dodatečné patentové ochrany, která může významně prodloužit tržní exkluzivitu. Polymorfní patenty tak představují účinný nástroj pro budování dalších patentových bariér a mohou dokonce omezit či blokovat prostor inovátora při uvádění alternativních pevných forem na trh. Tato dynamika zásadně ovlivňuje konkurenční prostředí a podtrhuje význam důkladného porozumění „skrytému světu“ polymorfie v moderním farmaceutickém vývoji.

1,3,5-TRIAZINES AND THEIR SYNTHETIC-BIOLOGY POTENTIAL

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Triazines are organic compounds with three nitrogen atoms in a six-membered aromatic ring, which is strongly deactivated by their presence. While 1,2,3-triazines (so-called vicinal) and 1,2,4-isomers (so-called asymmetric) are relatively less common than their symmetrical isomers – 1,3,5-triazines. Their preparation is based on two basic approaches: trimerization of nitriles or transformation of the substituents of the triazine nucleus.
Cyclotrimerization of nitriles is mainly applicable for the preparation of equally 2,4,6-trisubstituted 1,3,5-triazines. The preparation of unequally substituted 1,3,5-triazines is based on the conversion of substituents of the triazine nucleus, while the starting material is very often a 2,4,6-trichloro derivative - the so-called cyanuric chloride. This method has the advantage not only of variations in the addition of individual reagents, but also of the decreasing reactivity of intermediates with an increasing number of substituents.
The lecture will discuss individual 1,3,5-triazines that have found application in various areas of everyday life, but the most well-known are probably applications in medicine and especially in agriculture.

This work was supported by Ministry of education of the Slovak republic, the VEGA project 1/0385/25.

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FROM VARIABILITY TO PREDICTABILITY: A DOE-DRIVEN INSIGHT INTO PHARMACEUTICAL BLENDING

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Optimization of blending processes is a critical step in developing solid dosage forms, particularly for mixtures intended for direct tablet compression. Achieving uniform API distribution is essential for ensuring product quality, safety, and efficacy. As blending is influenced by multiple interacting factors, design of experiments (DoE) offers an effective framework for systematically understanding and controlling these variables.
This study presents a detailed DoE evaluation of a blending process for a bulk-produced mixture intended for direct compression. Experiments were performed in a 700 mL laboratory tumble blender using a mixing procedure previously identified as a cost-effective alternative to the industrial process. The design evaluated blend quality sensitivity to major critical process parameters (three fill levels, three mixing times, three API concentrations in the mixture, and two API batches). The blend quality was defined by API content uniformity, compressibility as rheological parameter, and particle size distribution. A quadratic D-optimal model in MODDE v13 selected 22 runs from 57 possible combinations, including three center points for evaluating model accuracy.
The DoE results provided several key insights. Analysis of API content uniformity across sampling locations revealed a pronounced segregation barrier, emphasizing the need to select process conditions that minimize segregation risk. The experiment showed excellent reproducibility, as all center-point blends exhibited similar concentration profiles. Blend compressibility proved to be a well-predictable parameter, whereas particle size distribution was not significantly affected by the tested conditions and remained consistent across blends. This study demonstrates that a well-structured experimental design is a powerful tool for achieving robust and predictive control of pharmaceutical blending processes, ultimately enabling more reliable and efficient development of direct compression formulations.

MITIGATING PROCESS-INDUCED DEGRADATION IN ACTIVE PHARMACEUTICAL INGREDIENTS VIA HIGH-ENERGY CO-PROCESSING AND STRUCTURAL EMBEDMENT

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Introduction
In pharmaceutical manufacturing, process-induced degradation remains a critical, frequently overlooked challenge. While industry routinely prioritises chemical compatibility, physicochemical transformations triggered by mechanical stress during unit operations often compromise the long-term stability of active pharmaceutical ingredients (APIs). This study investigated the interplay between processing energy, surface energetics, and chemical stability during the co-processing of a mechanosensitive model API.
Methodology

We evaluated two distinct dry co-processing technologies to assess how varying mechanical energy inputs influence formulation integrity. The API and polymeric excipient were co-processed, and structural and surface evolution were monitored via inverse gas chromatography (IGC), X-ray powder diffraction (XRPD), and scanning electron microscopy (SEM). Physical characterisation was coupled with post-process chemical stability profiling to monitor degradation kinetics.

Results

The first approach imparted substantially higher energy, inducing a rapid transition to a thermodynamically unstable amorphous state, yet resulted in less pronounced chemical degradation. This counterintuitive stabilisation stems from a unique structural incorporation mechanism. Instead of conventional surface coverage, finer API particles were deeply embedded within the larger excipient matrix, creating a composite shielding active domains from degradation. Conversely, the second technology showed process-induced degradation follows non-linear kinetics. Degradation occurred primarily during the initial 30 minutes before reaching a steady state, correlating with cyclic agglomeration and fragmentation.

Conclusion

Energy input and processing time are critical process parameters (CPPs) dictating API integrity. Identifying these CPPs reveals process-induced degradation early, allowing for proactive stability improvements before routine long-term and compatibility testing. Exploiting structural embedment mitigates this degradation, highlighting the necessity of integrating physical evaluations to engineer robust formulations.

Acknowledgements

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All materials were kindly provided by Zentiva, k.s.

TOTAL SYNTHESIS OF 16-F TAFLUPROST AS PROCESS IMPURITY

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Tafluprost (Taflutan®), a fluorinated prostaglandin $F_2\alpha$ analogue used for glaucoma treatment, is manufactured through a multistep process in which structurally related impurities may form under production conditions. Regulatory requirements demand identification, synthesis, and full characterization of such impurities to ensure robust process control and product quality.

In this work, we suggested developed a synthetic route that subsequently led to the targeted fluorinated process-related impurity detected during tTafluprost manufacturing, differing from the active pharmaceutical ingredient by an additional fluorine substituent at the C-16 position. A practical synthetic route was developed to access the impurity as

an analytically pure reference standard suitable for impurity qualification. The study provides insight into possible formation pathways under technological conditions and demonstrates how intentional impurity synthesis supports analytical validation, process optimization, and regulatory compliance in industrial prostaglandin production.

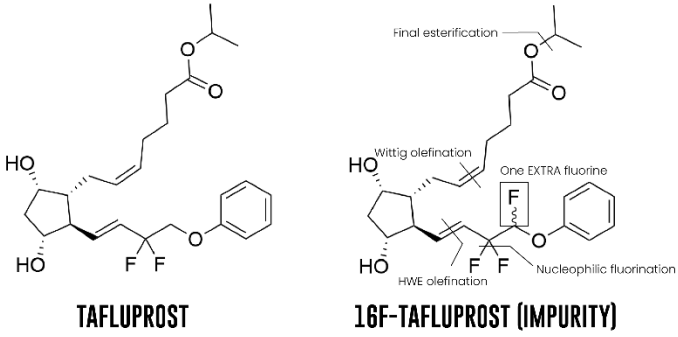

Figure 1: Structural difference between the prodrug tafluprost and its fluorinated process impurity 16F-Tafluprost.

Acknowledgements: the authors wish to acknowledge to Cayman Pharma, Neratovice, Czech Republic for coopertion.

MIHULKA – OBRANNÁ A PRAŠNÁ VĚŽ, ALCHYMISTÉ, IATROCHEMICI A FARMACEUTICKÁ FIRMA

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Válcovitá věž na Pražském hradě, zvaná Mihulka, je v povědomí široké veřejnosti spojována s alchymisty, kteří zde údajně sídlili v době Rudolfa II a prováděli svoje pokusy a obřady. Rudolfínskou dobu a zájem císaře o alchymii zpopularizoval film Martina Friče: Císařův pekař a pekařův císař, z roku 1951. Alchymistickou legendu použil i ing. Luboš Markovič při pojmenování svojí farmaceutické firmy v Opavě (Mihulka s.r.o.). Cílem tohoto příspěvku není bourání legendy, ale její kritická reflexe ve světle archeologických a literárních pramenů.
Ve své historii prošla věž Mihulka mnoha funkčními proměnami. Od obranné funkce přes kovolijeckou dílnu, laboratorium, skladiště střelného prachu, ubytovnu hradní posádky a kostelníků sv. Víta, až k dnešnímu muzeu Hradní stráže. Jméno Mihulka získala věž až v 19. století, jeho etymologie však zůstává nejednoznačná. Alchymistická tradice Mihulky vychází ze zápisu stavebního písaře Pražského hradu z roku 1609, podle něhož: …byla zbudována nová dřevěná chodbička k novému laboratoriu Jeho Císařské milosti… Podle

tohoto zápisu se nové laboratorium ale mělo přesně nacházet u Kulaté bašty a nikoliv přímo v ní. Navíc je třeba vzít v úvahu, že v rudolfinské době pojem laboratorium zahrnoval nejen místo pro alchymistické pokusy, ale také název pracovišť pro iatrochemické, destilační a jiné výrobny. Vzhledem k tomu, že přesná lokalizace alchymistických laboratoří na Pražském hradě není prokázána, tak působení alchymistů v Mihulce je historicky nedoložené. Z dnešního pohledu jde spíše o atraktivní, turisticky a komerčně využívanou legendu, která provází prohlídku hradního areálu. Spojení farmaceutické firmy Mihulka se stejnojmennou věží lze tedy chápat jako symbolické připomenutí kulturních a myšlenkových kořenů dnešní chemie a farmacie.

SYNTHESIS AND PRODUCTION OF PHARMACEUTICALS

POSTERS

SYNTHESIS OF AMPHIPHILIC DERIVATIVES OF DYE-BASED HETEROCYCLES AS POTENTIAL ANTINEOPLASTIC AGENTS

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Photodynamic therapy (PDT) represents a significant approach with multiple applications in clinical practice.[1] However, a major obstacle in the design and synthesis of new photosensitizers is their frequently limited solubility in aqueous media, which directly reduces their bioavailability. Particularly for dye-based heterocycles, addressing this pharmacokinetic parameter is even more urgent, as aggregation and lipophilicity fundamentally decrease their photophysical efficiency *in vivo*. Currently, 40% of commonly used drugs and up to 70% of newly synthesized molecules fall into the Biopharmaceutics Classification System (BCS) classes II and IV, which are characterized by low solubility[2]. Our work focuses on the synthesis of amphiphilic derivatives designed as potential antineoplastic agents. Targeted solubilization of model substrates in this concept is primarily realized by utilizing specific solubilizing building blocks and constructing block systems. Simultaneously, we are exploring new directions, such as direct solubilization on amino groups. Ongoing and future research goals include the completion of the designed series, its analytical quantification, and subsequent *in vitro* determination of cytotoxicity[3].

This work was supported by the VEGA project 1/0385/25.

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FROM MOLECULAR DESIGN TO BIOIMAGING TECHNOLOGY: Π-EXTENDED EHDPP D–A–D SYSTEMS WITH TUNABLE PHOTOPHYSICS

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Three symmetrical donor–acceptor–donor (D–A–D) systems based on N-alkylated 3,6-difuran-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (EHDPP) bearing differently π-extended furan-derived terminal units were designed, synthesized, and characterized.

Variation of the π-conjugated substituents markedly influenced intramolecular charge transfer. The compounds exhibited broad absorption between 300 and 620 nm, with bathochromic shifts up to 60 nm as conjugation increased.
They showed intense fluorescence in the 520–680 nm range with quantum yields of 30–79%, improving with extended π-systems. Solvent polarity had minimal impact on absorption, while emission displayed slight positive solvatochromism, indicating stabilization of excited states with donor–acceptor character.
Low-temperature measurements revealed better-resolved vibronic structure and longer excited-state lifetimes, particularly for the 2-phenylfuran-substituted derivative, attributed to suppression of nonradiative decay. DFT calculations confirmed increasing contributions of terminal groups to HOMO and LUMO orbitals from furan to 2-phenylfuran, consistent with stronger electron-donating ability.
Preliminary biological studies demonstrated high fluorescence stability and negligible cytotoxicity at concentrations suitable for cellular staining, supporting their potential as fluorescent probes. Overall, modification of terminal aromatic substituents proved crucial for tuning the electronic and photophysical properties of EHDPP derivatives for bioimaging applications.

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DYNAMIC TABLET DISINTEGRATION AS A TOOL FOR REVERSE ENGINEERING AND DESIGN OF GENERIC DRUGS

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Tablet disintegration is a critical step in oral drug delivery, directly influencing drug release and subsequent dissolution performance. Conventional pharmacopoeial disintegration and dissolution tests primarily provide endpoint or integral data, such as disintegration time or cumulative amount of drug release, offering limited insight into the structural evolution occurring during tablet breakup. Consequently, their ability to sensitively distinguish technologically different formulations remains restricted, which is particularly relevant in generic drug development.
This project explores dynamic tablet disintegration as a process-sensitive descriptor of tablet microstructure and technological history. The central hypothesis is that time-resolved particle size distribution data obtained during disintegration carry mechanistically relevant information not accessible through conventional testing. Static light scattering (SLS) is employed to continuously monitor the evolution of particle size distributions during tablet breakup, together with the total amount of particles dispersed in dissolution media, enabling the generation of characteristic “SLS fingerprints”.
Model formulations containing poorly soluble active pharmaceutical ingredients (APIs), including telmisartan as a pH-sensitive model compound, were prepared using predefined

technological scenarios reflecting industrially relevant variations in mixing order, excipient incorporation or lubrication level. Following basic pharmaco-technical characterization, tablets were subjected to time-resolved SLS monitoring under controlled, physiologically relevant conditions.
Quantitative descriptors characterizing fragmentation onset, disintegration mechanism and temporal evolution of size distributions were extracted and interpreted in relation to formulation design and processing history. Selected samples were further evaluated by dissolution testing to contextualize the dynamic disintegration data within conventional performance assessment.
The proposed methodology established dynamic disintegration profiling as a robust analytical tool for obtaining formulation characteristics additional to dissolution and composition testing. Therefore, its application in reverse engineering and rational design of generic formulations is promising and it can support more efficient formulation development and technology transfer in pharmaceutical practice.

METHODOLOGICAL EVALUATION OF API–EXCIPIENT INTERACTIONS THROUGH SURFACE ENERGY PROFILING

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Understanding surface interactions between an active pharmaceutical ingredient (API) and excipients is essential for predicting mixture behaviour, ensuring formulation robustness, and optimizing downstream processing. Surface energy (SE), specific surface area (SSA), and morphology can provide insight into the strength and nature of these interactions.
In this study, two batches of an API with different particle size distributions were investigated in combination with two commonly used excipients, Avicel® PH102 and Aerosil® 200, to evaluate physical compatibility in binary systems relevant to solid dosage formulations. Binary mixtures were prepared at two API loadings (low and high API content), using a standardized blending procedure in a 3D mixer to ensure reproducible mixing conditions. Surface characteristics of pure components and binary mixtures were characterized using inverse gas chromatography (IGC) to determine dispersion and specific components of SE, and the BET method to assess SSA. SEM imaging was employed to visualize particle morphology, coating phenomena, and the spatial distribution of API and excipients within the mixtures. Surface free energy (SFE) was then calculated by comparing experimentally measured surface energies of the binary systems with theoretical values derived from the pure components, allowing the extent of interfacial interactions to be quantified.
For API–Avicel mixtures, the dispersion component of SE lay between the values of the pure substances and decreased with increasing API content, while the specific component

showed a marked reduction, particularly for the finer API batch, indicating stronger interfacial interactions. In contrast, preliminary data for API–Aerosil systems suggested excipient-driven surface behaviour dominated by particle coating. SFE analysis for API–Avicel mixtures confirmed deviations from theoretical predictions, pointing to compositions with potentially improved rheological properties. Overall, the results demonstrate that SE–based characterization is a valuable tool for assessing excipient compatibility and for guiding formulation and process decisions in solid dosage development.

KYNURENIC ACID AMIDES IN TREATMENT FOR ALZHEIMER'S DISEASE

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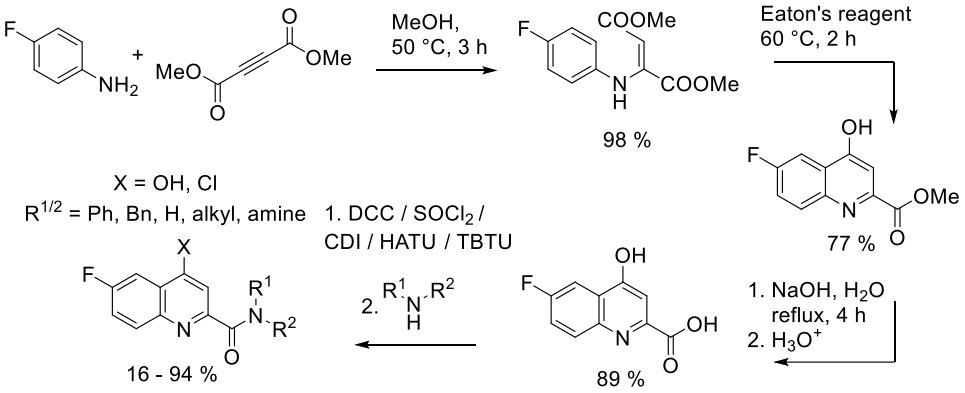
Alzheimer's Disease (AD) remains a leading neurodegenerative cause of dementia. Currently approved drugs primarily offer symptomatic relief by increasing acetylcholine concentrations (Donepezil, Rivastigmine, Galantamine) or mitigating excitotoxicity (Memantine). Conversely, recent disease-modifying therapies—specifically monoclonal antibodies such as Aducanumab, Lecanemab, and Donanemab—have demonstrated only modest efficacy in slowing neurodegeneration. To address the multifactorial pathogenesis of AD[1], the development of multi-target directing drugs (MTDDs) has emerged as a vital strategy. Kynurenic acid (KYNA) derivatives represent promising MTDD candidates due to KYNA's innate neuroprotective and anti-inflammatory properties; notably, it functions as an NMDA receptor antagonist similar to Memantine[2]. Derivatization of KYNA through the amidation with bioactive amines can enhance its MTDD character. Furthermore, the introduction of fluorine into the structure aims to optimize the unfavorable pharmacokinetic properties of KYNA, specifically its low aqueous solubility and poor BBB permeability. This work (Scheme 1) details the optimized synthesis of a KYNA ester and evaluates multiple amidation methodologies for the preparation of a novel KYNA amide series. Among the evaluated techniques for primary amines, direct acyl substitution from the KYNA ester proved most efficient, achieving a maximum yield of 94%. The resulting library is currently undergoing biological assessment for anti-Alzheimer properties in collaboration with the Slovak Academy of Sciences.



Scheme 1. Synthesis of KYNA ester and depiction of studied amidation methods.

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STUDYING THE DISSOLUTION KINETICS OF HIGH-MELTING DRUGS IN DOPED POLYMER MATRICES USING HOT-STAGE MICROSCOPY

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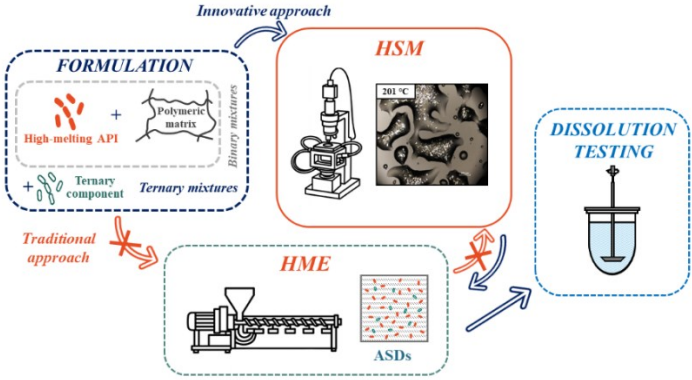
High-melting active pharmaceutical ingredients (APIs) represent a significant challenge in the development of amorphous solid dispersions (ASDs), as their fusion with the polymer matrix often requires temperatures close to the polymer's degradation temperature. This work establishes a systematic methodological framework for the rational design of ternary ASDs for such APIs. Hot-stage microscopy (HSM) represents a central component of this framework, providing mechanistic insight into temperature-induced phase processes that govern successful amorphization. HSM enables real-time observation of API melting, formation of homogeneous melts, early signs of phase separation, and the initial stages of dissolution within the polymer matrix. Quantitative image analysis revealed particle size evolution and dissolution-front progression, enabling differentiation between complete and partial dissolution across particle-size distributions. These data form the basis for identifying functional excipients capable of lowering processing temperature, improving miscibility, or promoting stable amorphization. The presented results constitute a key part of a broader research effort linking microscopically observed processes with practical manufacturability via hot-melt extrusion and with the dissolution performance of final formulations. Evaluation of selected ternary systems using HME, XRPD, and dissolution testing forms part of the broader research effort but lies beyond the scope of this contribution. Ultimately,

these results provide the mechanistic foundation for a comprehensive methodological framework integrating HSM, melt processing, and dissolution assessment to support the rational design of ternary ASDs for high-melting APIs.



TARGETED REMOVAL OF TRIFLATE SALTS AFTER DEPROTECTION OF *TERT*-BUTOXYCARBONYL PROTECTING GROUPS FROM THE GUANIDINE MOIETY

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Protecting groups constitute an essential and independent chapter of organic synthesis. Their general purpose lies in the strategic protection of reactive functional groups throughout a synthetic pathway.[1] Among the most widely used protecting groups is the *tert*-butoxycarbonyl (Boc) group. The Boc protecting group is extensively utilized in bioorganic chemistry for the protection of reactive primary and secondary amines during the synthesis of peptides, amino acids, and other natural products.[2] Its major advantages include cost efficiency, chemical stability (e.g., hydrogenation), and resistance to various reaction environments (e.g., basic conditions and nucleophilic reagents).[3] A notable limitation of the Boc group is the deprotection step, which is predominantly carried out using trifluoroacetic acid (TFA).[1,3] This process readily leads to the formation of trifluoroacetate salts, which may subsequently influence the chemical (e.g., solubility, reactivity), physical (e.g., density, conductivity), and biological properties of the resulting compounds.[3,4] From a biological perspective, trifluoroacetate salts may affect the activity of biologically active substances, particularly their stability and bioavailability.[5,6]

In the present study, we address the targeted removal of trifluoroacetate salts from the guanidine moiety of peptidomimetics. During a multistep synthetic pathway, the guanidine functionality was protected with two *tert*-butoxycarbonyl (Boc) groups. Final deprotection of both protecting groups resulted in the formation of two equivalents of trifluoroacetate, affording the corresponding bis(trifluoroacetate) salt. This issue was

successfully optimized by incorporating a neutralization step into the deprotection process, followed by purification *via* column chromatography. Through optimization of the deprotection process, we selectively obtained products in the form of the guanidine mono(trifluoroacetate) salt as well as the guanidine free base. The content of trifluoroacetate salts in compounds bearing the guanidine motif was quantified by ^{19}F NMR spectroscopy. Differences in the biological properties of guanidine-containing peptidomimetics in the form of the bis(trifluoroacetate), mono(trifluoroacetate), and free base are currently under further investigation.

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DECODING COMPACTION MECHANICS: INFLUENCE OF POWDER RHEOLOGY AND KINEMATICS ON TABLET AND API INTEGRITY

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Introduction
Developing solid dosage forms requires mastering the physical transformation of powders into compacts. While compression mechanics dictate tablet viability, the relationship between formulation flowability, dynamic compaction parameters, and resultant mechanical properties is complex. Furthermore, extreme physical stress during this transformation can compromise mechanosensitive active pharmaceutical ingredients (APIs). This study evaluates how formulation composition and processing kinetics govern tablet mechanics and subsequently influence chemical stability.

Methodology
A Design of Experiments (DoE) approach evaluated formulations with diverse flow characteristics. Using a benchtop compaction analyser, compaction load and dwell time were systematically varied. Key mechanical attributes, including plasticity, elasticity, and in-die frictional forces, were derived directly from comprehensive force-displacement profiles. Concurrently, process-induced API degradation was assessed via a stability-indicating chromatographic method (HPLC).

Results
Compaction load and dwell time profoundly dictated the mechanical profile of the compacts. Elevated loads and prolonged dwell times significantly amplified plastic deformation and ejection forces. Formulations exhibiting suboptimal flow experienced uneven die filling, exacerbating localised mechanical stress variations during compression. Crucially, these intensified physical stressors within the tablet matrix directly correlated with an increase in API degradation products.

Conclusion
Optimising tabletting kinematics and powder rheology is fundamental to controlling tablet mechanics. By rigorously profiling force-displacement data and ejection friction, formulators can define a safe compaction space. This proactive profiling ensures superior structural integrity whilst minimising the physical stressors responsible for API degradation, ultimately yielding mechanically robust and chemically stable solid dosage forms.

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UNEXPECTED CLEAVAGE OF N-N BONDS OF ALDEHYDE PENTAFLUOROPHENYL-HYDRAZONES – NEW SYNTHESIS OF NITRILES AND 2,3,5,6-TERTAFLUOROANILINE AND ITS ADDITION PRODUCT AMIDINES

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Pentafluorophenylhydrazones exhibit a broad spectrum of biological activities and have been described in the treatment of tuberculosis, malaria and anticancer agents and have also been identified as strong radical scavengers and their multitarget features have been combined as potential Alzheimer's disease (AD) therapeutics. Hydrazones were found to be effective inhibitors of amyloid beta fibril and oligomer formation as photodynamic therapy (PDT) represents a significant approach with multiple applications in clinical practice.[1-3] Our present work focused on the synthesis of 20 new aromatic aldehyde (naphthalene and acridine series) and heteroaromatic (N-substituted pyrrole, indole and acridine series) pentafluorophenylhydrazones and its cleavage of N-N bonds[1] in reaction with azide anion in DMSO[1] and simultaneously addition of formed 2,3,5,6-tetraflouroaniline with formed nitriles catalysed by NaH and produced new amidines. Ongoing and future research goals include the completion of the prepared series, and subsequent utilisation of newly prepared amidine derivatives for the synthesis of novel N-heterocyclic compounds with N-2,3,5,6-tetrafluorophenylgroup as new and perspective anti Alzheimer agents.

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ECONOMY OF THE CHEMICAL INDUSTRY IN NEW CONDITIONS

LECTURES

CHEMICAL TRENDS EU 2025

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SCHP ČR

Presentation covers current situation in EU chemical industry with decreasing competitiveness and closures of 9% capacitites in the last 3 years.
The EU27 chemical industry is facing a tough reality:
The competitiveness of the sector in Europe remains far below pre-crisis levels (2014-2019 average) driven by a combination of weak demand and uncompetitive energy prices. This is particularly an issue for commodity products and petrochemicals, where China has a competitive edge through large-scale production and low production costs.
Compared to the USA, European gas prices were 2.5 times higher throughout 2025, maintaining European producers at a competitive disadvantage. Since March 2022, the EU27 chemicals business environment has been facing a limited demand and declining business confidence, intensified by geopolitical uncertainty.
The EU27 chemicals capacity utilisation remains a key concern. It remains well below the EU's long-term average and has been well below the US average. The weak demand and declining business confidence continue to challenge the EU27 chemical industry.
The business trade environment in which European chemical companies are operating is exposed to high risks due to the unprecedented, global trade disruptions caused by US tariffs. EU27 chemical export values to the USA have continued to decline sharply since March 2025. By October 2025, export value had fallen by 60% compared with March 2025, dropping from €5.9 bn to €2.4 bn.

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IMPACT OF ENERGY CRISIS ON PERFORMANCE OF THE CZECH LARGEST CHEMICAL ENTERPRISES

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Introduction

Chemical industry in the Czech Repulic and Europe faced serious economic challenges in previous years. The energy crisis is mentioned as one of the reasons. There are government or union statistics quantifying the economic impacts which are mostly in the form of summarized results which could be influenced by some key players in the given industry. Therefore, the research aimed on individual business performance is conducted. It is exclusively focused on various areas of the chemical industry.

Methodology
To detect impacts of energy crisis, the quantitative research has to be conducted. First, various data sources, such as governmental statistics and annual reports publishing performance of inidividual enterprises, are collected. Second, the business financial performace is analysed with an empasis on profitability. It should be taken into consideration that there can be differences between sectors belonging to the chemical industry.
Results
The impacts of energy ciris on individual corporate performance are described and quantified. Discovered differences between the individual industry sectors are pointed out. Possible reasons for the observed differences are highlighted and discussed.
Conclusion
The findings show which industry sectors are more vulnerable and less flexible in the case of energy crisis. This kind of conclusion could have a practical benefit which businesses should be supported in the case of unfavour conditions. However, the research conducted has its limitations based on the size of data samples employed.

PURCHASING BEHAVIOUR IN THE CONSUMER CHEMICALS MARKET IN THE CONTEXT OF TRUST, CUSTOMER SCEPTICISM AND GREENWASHING

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The growing emphasis on corporate social responsibility (CSR) communication has intensified the debate about its effectiveness in shaping consumer purchase intentions, especially in environmentally sensitive sectors. The consumer chemicals sector is characterized by frequent environmental claims and increased public scrutiny, which increases the risk of perceived greenwashing and customer scepticism. In this study, we examine the determinants of purchase intention in the Czech consumer chemicals market by developing an integrative research model that links CSR communication, perceived greenwashing, customer scepticism, and purchase intention. Corporate social responsibility (CSR) communication is defined in the current literature as a strategic tool through which a company presents its economic, environmental, social, philanthropic, and ethical activities to key stakeholders with the aim of strengthening trust, legitimacy, and long-term competitiveness. Its quality is a significant determinant of brand perception and subsequent consumer purchasing behaviour. Greenwashing is understood as the deceptive or misleading communication of the environmental benefits of a product or company, for example by selective disclosure of information, unverifiable claims and certifications, etc., while ignoring significant negative impacts. At the same time, it can bring reputational risks from the difference between the declared and the actual.
The empirical part of the article presents the results of primary quantitative research conducted among consumers in the Czech Republic. The aim was to identify factors influencing purchase intention in the consumer chemicals sector, focusing on the role of

customer scepticism and perceived greenwashing as mediating factors that can weaken the positive effect of CSR communication on customer trust and subsequent purchase intention. Practical implications are formulated for managers in the consumer chemicals sector to mitigate scepticism and avoid the negative consequences of perceived greenwashing.

THE IMPORTANCE OF ENVIRONMENTAL ATTRIBUTES IN CONSUMER CHEMICAL PRODUCT OFFERINGS: A CONSUMER PERSPECTIVE

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With consumers' growing inclination toward sustainability—and, within that, toward environmental protection—their preferences when purchasing products, including consumer chemical products, are changing. For manufacturers of these products, it is essential to understand these shifts and adapt their offerings accordingly. To identify the importance of individual aspects of environmentally oriented consumer chemical product offerings, a primary quantitative survey was conducted among 400 Czech respondents selected through quota sampling. Data collection took place in the first half of 2023 through face-to-face interviews as well as an online questionnaire.

Statistical data analysis using descriptive methods showed that consumers consider the most important aspects to be those related to product composition, its use in the household, and its packaging. Consumers identified the following as key elements of an environmentally oriented offering: "providing clear and trustworthy product information on the packaging," "ensuring the product can be used and stored safely in the household," "the absence of hazardous substances in the product," and "packaging recyclability." Conversely, the least important for them are the facts that "the product does not contain animal-derived substances" and manufacturers' or retailers' communication about their socially responsible activities.

Statistical testing using the Friedman test further demonstrated that consumers also attach high importance to low product consumption and to reducing energy use during product use and storage. In the area of packaging, consumers additionally consider it important that the packaging ensures safe handling, fulfills a protective function, and prevents product waste.

BEHAVIORAL DETERMINANTS OF CSR COMMUNICATION: A SYSTEMATIC LITERATURE REVIEW OF THE THEORY OF PLANNED BEHAVIOR AND IMPLICATIONS FOR INDUSTRIES UNDER INCREASED REPUTATIONAL PRESSURE

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In the context of growing emphasis on corporate social responsibility (CSR) and sustainable industrial transformation, increasing attention is being paid to the behavioral mechanisms that shape stakeholders' responses to CSR communication. Many firms across industrial sectors, particularly those operating in industries exposed to heightened reputational pressure—face a persistent gap between declared responsible activities and their actual acceptance by the market.

The aim of this paper is to systematically analyze how the Theory of Planned Behavior (TPB) has been applied in research on CSR, sustainability, and ESG, and to identify its contribution to the management and communication of responsible corporate strategies across industries. The study is based on a systematic review of 294 peer-reviewed journal articles published between 2016 and 2025 in Q1 and Q2 journals. Using the PRISMA methodology and bibliometric analysis conducted with VOSviewer software, dominant research themes and the most frequent TPB model extensions were identified, particularly those incorporating moral norms, environmental attitudes, value-based constructs, and trust-related variables.

The findings reveal a strong methodological focus on behavioral intentions rather than actual behavior and highlight structural weaknesses in the current evaluation of CSR communication effectiveness. The study provides a general behavioral framework for understanding stakeholder responses to responsible corporate strategies, applicable across sector-specific contexts, including industries characterized by higher regulatory and reputational scrutiny.

From the perspective of economics and management in the chemical and process industries, the paper emphasizes the need for systematic integration of behavioral determinants into CSR communication design and strategic management to reduce the gap between declared responsible activities and their real-world impact.

DECEPTIVE COMMUNICATION AND CRISIS REPUTATION MANAGEMENT IN THE CHEMICAL INDUSTRY

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The article addresses the issue of deceptive communication and crisis reputation management in the chemical industry, a sector that has long been exposed to an elevated level of reputational risk due to the environmental, safety, and ethical externalities inherent in its operations. Reputation is conceptualized as a socially constructed, multidimensional evaluation of a company by its key stakeholders, determining its legitimacy, competitiveness, and long-term sustainability. Reputational risk is understood as the potential disruption of this evaluation resulting from discrepancies between declared corporate values and actual practices, with the nature and quality of corporate communication playing a pivotal role in this process. The paper briefly outlines the importance of ethical, authentic, and transparent communication in building trust and identifies typical unethical and non-transparent communication techniques that may contribute to reputational erosion. It further reflects literature-based principles of communication management in reputational crises, particularly emphasizing accountability, message consistency, and the implementation of corrective measures.
The empirical part of the study presents the results of primary quantitative research conducted among respondents from the public. The objective was to examine which unethical and non-transparent communication techniques the public has encountered in relation to chemical industry companies and to identify which crisis communication strategies are perceived by respondents as the most effective in defending corporate reputation. Based on the data obtained, recommendations for reputation management practice in the chemical industry are formulated. The study contributes to the scholarly discourse on the ethical boundaries of corporate communication in sectors with significant societal impact and underscores the importance of a transparent and responsible approach as a key prerequisite for long-term reputational stability.

SUSTAINABLE PROJECT MANAGEMENT AND INDUSTRY 5.0: ANALYSIS OF APPLICATION AND BARRIERS IN THE CZECH CHEMICAL INDUSTRY

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Presented research is focused on the integration of sustainable project management (SPM) and the Industry 5.0 concept within the chemical industry environment in the Czech Republic. The objective of this research was to identify the extent of application of these

principles, the motivations for their implementation, and the key barriers preventing deeper integration. The research was conducted combining quantitative and qualitative approaches.

The quantitative research analysed a dataset of 234 grant projects financed or co-financed by EU Funds implemented by members of the Association of Chemical Industry of the Czech Republic across programming periods from 2007 till 23.2.2025. The results indicate that while sustainable projects have been only 82 projects in absolute numbers, they represent nearly a two-thirds majority of all received grants (5.38 billion CZK) from 8,61 billion CZK of total amount. The sustainable projects are focused mainly on energy savings, building insulation, and emission reduction.

The qualitative phase, based on in-depth interviews with Czech and foreign experts and managers from chemical industry, revealed a significant discrepancy between high awareness of sustainable methods and their superficial application in actual corporate practice. The primary identified barriers include high initial costs, low customer willingness to pay a "sustainability premium," and the technological complexity of chemical processes.

In conclusion the research formulates recommendations for the strategic alignment of projects with the organization's ESG goals, strengthening education in the field of sustainability, ESG principles and for project managers in the SPM area. It also recommends more active use of public subsidy titles to finance the transformation of the chemical sector towards a circular economy and climate neutrality. And based on improved knowledge, to focus more on these strategies and to use private financial resources to accelerate this transformation.

CASE STUDIES OF INDUSTRY 4.0 IN THE CZECH CHEMICAL INDUSTRY

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Introduction

Industry 4.0 can be understood as the fourth independent industrial revolution coming with significant technological shifts leading to the replacement of human labour by modern machines. These investment actions are connected with enormous cash expenditures for which many business do not have the resources. Although it is assumed that the Industry 4.0 concept would probably have a more negligible impact on the chemical industry than on other industry branches it is emphasized that without such activities there is the risk of losing business competitive advantage. Therefore, the research aimed on implementation of Industry 4.0 is conducted. It is exclusively focused on various areas of the chemical industry.

Methodology

To detect case studies of Industry 4.0, the desk research has to be conducted. Data sources mostly consist of webpages and annual reports of individual companies in which enterprises present realized or planned investment projects. The data is not structured

and uniform, and therefore it is necessary to manually proceed it with an emphasis on a qualitative aspect. The obtained projects are classified according to selected criteria focused on a project size, aim, and content.

Results

Collected investment projects belonging to Industry 4.0 are presented. These projects are described and summarized accoring to the selected criteria. This shows the development trends of Industry 4.0 in the chemical industry in the Czech Republic.

Conclusion

The findings show current and previous implementations of Industry 4.0 in the chemical industry in the Czech Republic. This kind of conclusion has a practical benefit for different groups including government policy makers, union representatives, and corporate managers. However, the research conducted has its limitations based on data availability and data uniformity.

SUSTAINABLE STRATEGIES AND CORPORATE SOCIAL RESPONSIBILITY IN THE BEVERAGE INDUSTRY

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Modern society faces complex environmental, social, and health challenges that require a transformation of business approaches. In this context, the non-alcoholic beverage industry is under increasing pressure, particularly due to high water consumption, packaging waste generation, and the links between the consumption of sugar-sweetened beverages and chronic diseases. Growing expectations from regulatory authorities, financial institutions, and consumers are leading companies to implement sustainability, CSR, and ESG concepts that integrate economic performance with environmental and social responsibility.

The aim of this study is to systematically map the development of research focused on sustainability, CSR, and ESG strategies in the non-alcoholic beverage sector during the period 2016–2025. The study applies a combination of bibliometric analysis and manual content interpretation of 194 articles indexed in the Web of Science database (SSCI, Q1–Q2). The VOSviewer software was used to visualize relationships among keywords and to identify thematic clusters.

The results identified four dominant thematic areas: (1) sustainable business practices and supply chain management, (2) circular approaches and environmental efficiency, (3) innovation and corporate social responsibility, and (4) ethical efficiency and eco-labeling. The research is geographically concentrated mainly in developed economies, while developing regions remain underrepresented. The analysis also indicates that corporate strategies are often declarative in nature and lack systematic evaluation of the measurable impacts of ESG policies.

The study contributes to a deeper understanding of research trends in the beverage sector and identifies directions for future research, particularly in the areas of empirical impact assessment, behavioral aspects of consumption, and the geographical diversification of research.

THE ECONOMIC RELEVANCE OF BIODIVERSITY FOR CHEMICAL COMPANIES

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Current global biodiversity loss represents a significant systemic risk for industrial enterprises, particularly within the chemical sector, transcending traditional corporate social responsibility. This article investigates the bidirectional relationship between biological diversity and business continuity. The first section categorizes critical economic threats stemming from ecosystem degradation, specifically focusing on the disruption of raw material supply chains, escalating regulatory pressures under the EU Green Deal, and the rising shadow costs of substituting lost ecosystem services, such as natural water purification and climate regulation. The core of the article determines current mitigation measures implemented in industrial practice, ranging from site-specific technical solutions—such as the ecological restoration of industrial brownfields and integrated water management—to high-level strategic tools, including ESG-linked biodiversity metrics. Furthermore, the article presents successful and widely adopted solutions from business practice, illustrating their direct impact on the financial performance of companies.

Identification of selected elements of higher education reform in the Slovak Republic aimed at increasing the productivity of industrial production.

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In October 2025, the reform of the Higher Education Act came into force in Slovakia. An important element is the introduction of new options for formal education and the use of the possibility of changes in the creation and scope of educational programs at universities. The paper identifies the possibilities offered by the aforementioned change to the Higher Education Act in direct connection with the quality and scope of competencies of university graduates, which potentially affect productivity in industrial production.
The paper uses methods of comparing the previous state of universities and changes after the amendment to the Higher Education Act. These changes reflect the conditions of Industry 4.0 and, at present, we can say that also the approaching Industry 5.0. The identification of selected elements in the paper points to the needs for new knowledge and skills that a graduate of technical fields should achieve.

ECONOMY OF THE CHEMICAL INDUSTRY IN NEW CONDITIONS

POSTERS

ECONOMIC COSTS OF REACH/KKDIK COMPLIANCE AMONG SMEs IN TÜRKİYE: A REFLEXIVE THEMATIC ANALYSIS

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REACH and its Turkish equivalent KKDIK impose extensive data generation, risk assessment, and registration obligations on chemical substances placed on the market. While these frameworks aim to ensure a high level of protection for human health and the environment, their procedural and financial complexity may create disproportionate compliance burdens for Small and Medium-Sized Enterprises (SMEs). This study investigates the economic costs emerging during REACH/KKDIK compliance processes among SMEs operating in Türkiye's chemical sector. A qualitative research design was adopted based on semi-structured interviews conducted with regulatory affairs professionals, environmental engineers, and compliance managers employed in SMEs. Data were analysed using Reflexive Thematic Analysis, including phases of data familiarisation, initial coding, theme construction, and interpretation of economic implications. Findings indicate that compliance-related decision-making within SMEs is primarily driven by cost considerations, exacerbated by high data-sharing fees, lack of in-house toxicological expertise, and limited administrative capacity at the national regulatory level. Although regulatory compliance functions as a prerequisite for maintaining export competitiveness, the one substance, one registration principle may generate structural asymmetries favouring large multinational firms over local SMEs. These findings suggest that compliance costs operate as a structural barrier to market participation, reshaping SMEs' ability to access European markets and chemical supply chains.

GLOBAL PERSPECTIVE OF THE SOCIAL DIMENSION OF SUSTAINABILITY IN SUPPLY CHAINS: A BIBLIOMETRIC AND CONTENT ANALYSIS

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Global supply chains are undergoing significant changes that are reshaping corporate management practices. Increasing pressure from regulators, investors, and the public is driving companies toward greater transparency and accountability. While environmental performance is already commonly measured and integrated into strategic decision-

making, the social dimension of sustainability remains less clearly defined and more difficult to measure. This dimension includes occupational safety, employee health protection, human rights, equal treatment, and the impacts of business activities on local communities. Inadequate management of these areas may pose both reputational and economic risks.

The aim of this study is to systematically map the development of research focused on managing social aspects in supply chains across industries. The study identifies the main research streams, theoretical foundations, and geographical distribution of publications, while also highlighting key research gaps.

The research is based on a systematic literature review conducted in accordance with the PRISMA protocol. The study draws on articles retrieved from the Web of Science (SSCI) database, published between 2021 and 2025. From an initial 1,724 records, 391 articles were selected for detailed analysis after applying predefined criteria. The study combines bibliometric analysis with content analysis of the selected studies.

The results indicate that social topics are often addressed only within the broader framework of sustainability and are rarely directly linked to firms' economic performance. Moreover, the research is geographically concentrated primarily in countries of the Global North. The impacts of digitalization and automation on employees are also insufficiently explored. The study provides an overview of current knowledge and proposes directions for future research aimed at improving the operationalization of social sustainability in supply chain management, particularly in the chemical industry, where social risks are closely interconnected with safety, regulation, and the high process intensity of production.

FINANCIAL PERFORMANCE AND RESILIENCE OF THE SLOVAK CHEMICAL INDUSTRY: EVIDENCE FROM DUPONT DECOMPOSITION AND BANKRUPTCY PREDICTION MODELS

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This study examines the financial performance and stability of selected companies operating in the Slovak chemical industry during the period 2018–2023. The research focuses on enterprises established in Slovakia and operating under Slovak accounting and tax regulations. Financial data were obtained from financial statements (balance sheet, profit and loss statement, and notes) available in the Register of Financial Statements. The analysed sample consists of large companies acting as suppliers within the chemical industry. The selected period captures financial development before the COVID-19 pandemic, during the crisis, and in the subsequent recovery phase.

The study applies the DuPont system of financial analysis to identify the main determinants of return on assets (ROA) and return on equity (ROE). Pearson correlation analysis is used to examine relationships between key financial indicators. Financial stability is further assessed using the Altman Z-score model and the IN05 bankruptcy prediction index.

The results indicate that ROA is primarily driven by profitability of sales (EBIT/revenues), which shows a strong positive correlation in most analysed years. In 2020, declining demand in key industrial sectors reduced revenues and profitability and weakened the utilisation of production capacities. This increased the volume of tied assets and negatively affected asset turnover and profitability. In the following years, companies sought to stabilise performance mainly through improved profit margins. ROE was strongly influenced by ROA, while the impact of financial leverage varied during the analysed period.

Predictive models confirm a deterioration in financial stability during the pandemic, followed by gradual recovery from 2021. However, rising energy prices and input costs again pressured profitability in 2022–2023. The findings highlight key financial factors shaping the resilience of companies in the Slovak chemical industry during periods of economic disruption.

MATERIALS AND PROCESS ENGINEERING

LECTURES

LASER SHOCK PEENING FOR ENHANCED FATIGUE AND TRIBOCORROSION PERFORMANCE OF CONVENTIONAL AND ADDITIVELY MANUFACTURED METALLIC ALLOYS

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Metallic materials are widely used in demanding applications ranging from aerospace and biomedical implants to chemical processing equipment, where fatigue, wear, and corrosion often limit service life. Surface engineering techniques that can simultaneously improve mechanical durability and chemical resistance are therefore of great interest. In this lecture, we present an integrated study on the effects of Laser Shock Peening on conventional and additively manufactured alloys, including Ti-6Al-4V, Ti-6Al-7Nb, SS316L, and Steel 304. The discussion covers fatigue behavior at room and elevated temperatures, fretting wear, and tribocorrosion under biological and chemically aggressive environments. Key findings highlight how LSP induces compressive residual stresses and microstructural modifications, leading to significant improvements in fatigue life and resistance to tribocorrosion and fretting wear. Differences in response between conventional and additive manufactured materials are emphasized, providing insights into microstructure-dependent performance. The lecture will also address future directions for combining additive manufacturing with surface treatments to develop metallic components with tailored properties for industrial and biomedical applications. By bridging fundamental mechanisms and practical performance, this work illustrates the potential of LSP to extend the durability and reliability of advanced metallic systems.
Keywords: *Laser Shock Peening; Fatigue; Tribocorrosion; Additive Manufacturing; Metallic Alloys*

MECHANICAL ALLOYING AS A WAY TO NON-CONVENTIONAL MATERIALS

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Mechanical alloying is a process in which solid solutions or compounds are formed during high-energy milling. During the process, particles are mechanically interconnected by plastic deformation and the resulting particles are simultaneously fragmented. The kinetic energy transferred to the milled powder also causes local heating. This creates, among other things, conditions for the formation of intermetallic compounds, including metastable ones, which otherwise do not form during conventional metallurgical

operations (melting, casting, heat treatment, etc.). Due to the severe plastic deformation during grinding, the resulting powder has a very fine-grained structure. If the powder is subsequently suitably compacted so as to avoid significant grain coarsening, the resulting products achieve significantly better mechanical properties than materials produced by conventional technologies.
This work presents the possibility of using mechanical alloying in the preparation of several technically important materials – high-temperature intermetallic materials based on FeAl and TiAl, hard intermetallic composites and quasi-crystalline Al-Cu-Fe phases.

This research was financially supported by Czech Science Foundation, project No. 23-05126S.

NEW LOW TEMPERATURE SYNTHETIC METHOD FOR PREPARATION OF TELLURIDES NANOPARTICLES FOR POTENTIAL SENSORIC APPLICATIONS

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Keywords: organometallic precursors, tellurides, nanoparticles, TEM, LA TOF MS

Nanoparticles can offer an alternative approach to fabricate phase-change materials. The chemical synthesis of GeTe nanoparticles using organometallic precursors exploits high-boiling solvents and relatively high temperatures (close or even above crystallization temperatures) and by the reduction of the tellurium source (for example Na_2TeO_3 or $TeCl_4$)[1] together with (semi)metallic source (GeI_2 or $SnCl_2$)[2] at the elevated temperatures (above 150 °C) for several hours. There are also reports showing that similar procedure in the presence of second metallic source (for example $InCl_3$, $In(NO_3)_3$) or even the metallic nanoparticles (NPs) may provide doped telluride materials.[3] Nanoparticles can offer an alternative approach to fabricate films of phase change material. Contrary, the reports of chemical synthesis at room temperatures are in fact unknown.
The aim of this work is preparation of tellurides nanoparticles of main group metals by low temperature synthetic method by the help new organometallic precursors. The main part will be focused on different preparation methods and characterization GeTe nanoparticles for protential sensoric applications. The characterization of prepared nanomaterial was performed on the basis of high-temperature X-ray diffraction, transmission electron

microscopy, LA TOF mass spectrometry, X-ray diffraction, Raman spectroscopy and dynamic light scattering.

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INVESTIGATION OF THE INFLUENCE OF DOPING TELLURITE GLASSES WITH CUO AS COLORANT FOR DIRECT LASER WRITING

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Tellurite glasses are promising materials for optical and photonic applications due to their high refractive index, high stability, broad infrared transparency, and ability to incorporate dopant ions. This work focuses on the preparation, characterization, and direct laser writing of tellurite glasses with the composition $80TeO_2$–(20–x)ZnO–xCuO, where x = 0–4 mol%. The aim was to evaluate the influence of CuO addition on the structural, physical, and optical properties of these materials and to assess their suitability for applications in direct laser writing using different wavelengths.
Elemental composition was analysed via SEM–EDX and XRF. Bulk density, glass transition temperature, softening point, and coefficients of thermal expansion were measured. Optical behaviour was studied using UV–Vis and infrared spectroscopy, focusing on absorption changes with CuO content and interaction with laser radiation.
Direct laser writing was performed with continuous-wave lasers at 455 nm, 785 nm, 1064 nm, and 10.6 µm. Colourless undoped glasses were responsive only to the 10.6 µm laser. CuO addition created colour centres by a new absorption band with maximum at 810 nm.

Laser irradiation produced surface modifications, including microlenses up to 7 μm in height and craters deeper than 6 μm on the surface of $80TeO_2$–16ZnO–4CuO glass exposed to the 1064 nm laser.
The results demonstrate that CuO addition improves optical absorption and coloration, enabling efficient laser processing, while thermomechanical and structural properties remain largely unchanged.
This work was supported by the CAS project 25-15635S.

STRUCTURE AND PROPERTIES OF ELECTROFORMED BIODEGRADABLE IRON

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Among biodegradable materials for temporary implants (e.g., stents or bone scaffolds), iron and its alloys are promising due to their good mechanical strength and biocompatibility. However, their corrosion rate is much lower than required for clinical applications, meaning degradation must be accelerated to avoid long-term persistence in the body.
The corrosion rate can be increased by modifying the manufacturing process. Electroforming, unlike conventional methods such as casting, produces electroformed iron (EFI) with a finer grain structure. The higher density of grain boundaries then provides more active sites for corrosion, thereby accelerating degradation.
EFI was prepared on a polished TiAlV plate from a solution containing $FeCl_2$, $CaCl_2$, sodium saccharin, and sodium dodecyl sulfate at 90 °C for 8 h. Corrosion behavior was evaluated by long-term immersion testing for two months in simulated body fluid solution (SBF). Mechanical properties were evaluated by tensile testing and microhardness measurements.
The results showed that EFI exhibited an 18-fold higher corrosion rate (0.003 vs 0.055 mm y^{-1}) compared with conventionally processed pure iron. EFI demonstrated nearly twice the yield strength of pure iron, while microhardness measurements revealed approximately a twofold increase in hardness.
Electroforming significantly increased the corrosion rate and represents a promising approach for modifying biodegradable iron; however, the achieved corrosion rate is still insufficient for practical biomedical applications. In future work, suitable alloying elements (e.g., Mn, Zn) may be incorporated to further accelerate the corrosion rate of electroformed iron.
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IN SITU TEM AND MOLECULAR DYNAMICS ANALYSIS OF SINTERING MECHANISMS IN NICKEL NANOPARTICLES

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The sintering behavior of nickel nanoparticles (Ni NPs) was investigated using a combined experimental and computational approach that integrated in situ transmission electron microscopy (TEM) annealing with molecular dynamics (MD) simulations. Particular attention was devoted to the mechanisms initiating sintering and the factors governing particle interaction and coalescence during thermal treatment. In situ TEM observations provide direct insight into temperature-induced morphological evolution, revealing a gradual increase in particle diameter from an initial mean size of 8 nm as the temperature was raised from room temperature to 850 °C. At elevated temperatures, the particles ultimately merge into larger aggregates. This behavior is driven by the tendency of the system to minimize its total surface energy, promoting the formation of larger, more compact structures with reduced overall surface area. MD simulations offer atomistic insight into the processes underlying these transformations and show the formation of necks even at room temperature. In contrast, the TEM observations exhibit no pronounced structural changes below 300 °C. Taken together, both the experimental results and the simulations indicate that surface diffusion is the dominant mechanism responsible for neck formation and growth between Ni NPs during sintering.

EFFECT OF HEAT TREATMENT ON THE MICROSTRUCTURE AND MECHANICAL PROPERTIES OF NITI–TIC COMPOSITE FOR BALLISTIC PROTECTION APPLICATIONS

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In the context of the growing instability of the global geopolitical situation—a trend further accelerated by events since the beginning of 2026—investment in defense technologies is becoming a vital tool for ensuring both national and alliance security. Innovations in the protection of human resources and key technological systems represent a significant factor in maintaining technological superiority in the defense sector.
Currently, so-called hard body armor is the most widespread among police and military units. This type of ballistic protection consists of a macro-composite made of a steel plate, ceramic reinforcement, and layers of high-strength textiles supplemented with anti-traumatic materials. Although this design is effective at dissipating the kinetic energy of a projectile, it is susceptible to degradation due to environmental conditions, particularly changes in temperature and humidity, which can lead to a deterioration of its performance characteristics.

A possible alternative is a NiTi-based composite reinforced with TiC particles. However, the preparation process leads to a decrease in the material's plasticity, which can be influenced by appropriately selected heat treatment conditions. In this work, therefore, in addition to the microstructure, the effect of heat treatment on the hardness and compressive strength of the prepared samples was also investigated.

This work was financially supported by the Czech Science Foundation (project No. 25-15757S,Plasma valorization of waste into cutting-edge cermet composites for high kinetic energy dissipation).

SCALABLE MAGNETRON-SPUTTERED COPPER-BASED 3D NANOSTRUCTURES

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Porous copper nanostructures are highly attractive for Al-based battery systems and catalytic applications, where a large surface area and well-controlled nanoscale morphology strongly influence reaction performance. Magnetron sputtering offers a scalable route to engineer such nanostructures, as geometry, thickness, and porosity can be directly tuned through deposition parameters. In our work, we fabricated several types of porous, tree-like Cu nanostructures using a gas aggregation source for nanoparticle formation, complemented by co-sputtering to incorporate additional elements during growth, enabling precise control over composition.

To investigate thermal stability and phase evolution, we combined in situ TEM annealing with complementary TEM measurements on free-standing films and cross-sectional lamellae. A key finding is that annealing triggers phase transformations while largely preserving the overall morphology. In samples containing aluminum, thermal treatment resulted in the formation of the intermetallic Al_2Cu phase without disrupting the nanoscale architecture. These results suggest that combining composition control during growth with post-deposition annealing provides a general strategy for producing intermetallic nanostructures that may not be achievable through direct sputtering alone.

Overall, this approach demonstrates that integrating nanoparticle sputtering, co-sputtering, and controlled annealing enables the fabrication of Cu-based nanostructures with tunable geometry and composition – including intermetallic phases – while maintaining their nanoscale morphology.

NUMERICAL SIMULATION OF MAIZE KERNEL POPPING – POPCORN PRODUCTION IN FLUIDIZED BED REACTOR

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Popcorn is one of the most popular snack products worldwide and represents a simple yet illustrative example of a thermally driven food processing operation. The objective of this work is to use popcorn production as an understandable model system for studying the behaviour of a fluidized bed reactor. Maize kernel and popcorn have different volume which makes it easy to separate them in air stream so fluidized system was chosen for that reason. Maize kernel is a heterogeneous structure (germ, pericarp, endosperm) with thermal and mass transfer properties that vary by variety and moisture content. To enable modelling, the kernel was approximated as a two-component sphere (dry matrix and water), allowing for 1D numerical analysis of coupled heat and mass transfer. Based on the known temperature required for kernel popping, the model allows simulation of continuous popcorn production.

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ASSESSING THE OPTIONS FOR C3 FRACTION DISTILLATION INTENSIFICATION BY ITS HYBRIDIZATION

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C3 fraction distillation belongs to very energy-intense processes, consuming heat equivalent of up to 2 tons of water steam per ton of processed feed and discharging comparable amount of heat to cooling water in the condenser. Conventionally, high-pressure or low-pressure C3 splitter design is adopted with either external heat delivery and extensive cooling water use, or the integration of a heat pump allowing for column operational pressure decrease. Design hybridization by a pre-separation process integration offers an interesting means of process intensification, reusing most of existing assets. This study is dedicated to exploring the techno-economic features of such design change, employing a membrane-based pre-separation step, focusing rather on possible feed processing rate increase than the possible decrease of operational expenses at feed processing rate unchanged. Study results indicate that the proposed hybrid process can be economically viable provided the related membrane research and development

proceeds yield reasonable membrane cost and improved durability and retained separation ability over the operational period of ten years.

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SCALE-UP OF NITROGEN-DOPED GRAPHENE FOR HIGH-PERFORMANCE SUPERCAPACITORS

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Two-dimensional carbon materials are widely considered promising electrodes for next-generation electrochemical energy storage. However, their industrial deployment remains constrained by the lack of scalable and reproducible production routes for functional graphene derivatives.
Here, we present a wet-chemistry scale-up of a fluorographene-derived nitrogen-doped multilayer graphene developed for high-performance supercapacitor electrodes. The material combines nitrogen doping of 16 at.% with a high mass density of 2.8 g cm^{-3}, enabling significantly improved volumetric electrochemical performance compared to conventional activated carbon electrodes used in commercial supercapacitors.
The material is protected by patents and currently represents the only reported fluorographene-derived nitrogen-doped multilayer graphene produced at a multi-kilogram scale.
The synthesis process involves large-volume exfoliation of fluorinated graphite, controlled nitrogen functionalisation, multistep purification, and spray-drying to produce a stable powder suitable for electrode fabrication. Current process development secures batch production up to 3 kg of final material.
Key engineering bottlenecks arise primarily from large-scale exfoliation and the purification workflow. Ongoing optimisation focuses on improving exfoliation efficiency and accelerating washing and desalination through scalable filtration and process intensification strategies.
This work focuses on the practical chemical engineering challenges associated with translating advanced graphene materials from laboratory synthesis to industrial production and demonstrates the potential of the dense nitrogen-doped graphene derivative to enable compact, high-performance supercapacitors for demanding applications.

CIRCULAR DECONVOLUTION VIA MOLLIFICATION FOR RTD RECOVERY IN CHEMICAL ENGINEERING

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The recovery of Residence Time Distributions (RTD) from blurred and noisy experimental observations is a ill-posed inverse problem in chemical reaction engineering. To tackle such periodic inverse problems, this work characterizes a variational mollified circular deconvolution method. By utilizing approximate unities, the proposed approach provides controlled spectral regularization, offering a robust, theoretically grounded alternative to standard techniques. A central focus of this contribution is the rigorous mathematical characterization of the method. We demonstrate that the regularization functional admits a unique minimizer and that the associated stability condition is satisfied whenever the mollifier is nonnegative and even. Furthermore, we establish the strong consistency of the mollified reconstruction, proving its convergence to the exact uncorrupted solution as the regularization parameter approaches zero. To formalize the method's performance under realistic conditions with noisy observational data, we comprehensively analyze its asymptotic properties. This includes deriving pointwise, Lp, and Besov-Nikoslkii convergence rates, and explicitly bounding the noise amplification for cases involving polynomial and exponential kernel decay. Finally, we connect this theoretical framework to chemical engineering by applying our reconstruction formula to a numerical example of RTD recovery. By solving this challenging inverse problem, our method offers a reliable, mathematically grounded tool for industrial chemical analytics.

SIMPLIFIED MODEL OF WALL-TO-BED HEAT TRANSFER IN LIQUID-SOLID FLUIDISED BED

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The heat transfer from the tube wall to the liquid flowing through a layer of fixed particles is studied numerically using the finite element method (FEM). The flow of liquid through a layer of fixed particles, with layer porosity corresponding to a fluidised bed, is used to imitate wall-to-fluidised bed heat transfer. The numerical simulation is performed with different spatial configurations of the particles in the tube. The spatial configuration of the particles has considerable influence on the results of the numerical simulation of heat transfer. The results of the simulation are compared with experimental data from the

literature obtained from heat transfer measurement in the liquid-solid fluidised bed system. The heat transfer coefficients calculated from the simulation results are lower than the experimental values, but in a certain spatial configuration of particles, there is a similar trend in the data.

CHARACTERIZATION OF PLAIN AND INFILTRATED TiAlV SCAFFOLDS

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The TiAlV scaffolds are widely studied for medicinal application. Scaffolds used in this study were prepared by SLM additive manufacturing technique. Consequently, they were infiltrated by Zn-based alloy. Both, plain and infiltrated scaffolds were studied by optical and scanning electron microscopy and by means of neutron tomography. The main task of this study is to find infiltration conditions with none or negligible formation of intermetallic phase on the boundary between TiAlV reinforcement and Zn matrix.

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CSPBBR$_3$ HYBRID MATERIALS: FROM POLYMER COMPOSITES TO BOROPHOSPHATE GLASS HOSTS

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Hybrid materials combining lead-halide perovskites with polymer matrices represent a promising class of luminescent systems for photonic and scintillation applications. In this work, we investigate composite systems based on $CsPbBr_3$ particles embedded in polystyrene together with ZnO–polystyrene structures, focusing on their optical response, defect-related processes, and charge-transfer mechanisms.

$CsPbBr_3$ micro- and nanocrystals exhibit strong excitonic emission around ~2.4 eV and ultrafast luminescence decay, making them attractive for fast photonic detectors and scintillation materials. However, their stability and optical performance are strongly influenced by surface defects and environmental interactions. Embedding the perovskite particles into a polystyrene matrix represents an effective approach to modify charge trapping processes, passivate surface states, and improve environmental stability. Previous studies have shown that polymer encapsulation can significantly influence luminescence decay dynamics and suppress defect-related paramagnetic centers.

In addition to $CsPbBr_3$–polystyrene composites, ZnO–polystyrene systems were investigated as complementary hybrid materials with strong UV absorption and defect-related luminescence. The optical properties of these polymer–inorganic hybrids were analyzed using photoluminescence and complementary spectroscopic methods to evaluate the role of interfaces and defect states in energy transfer processes.

For comparison, $CsPbBr_3$ nanocrystals embedded in borophosphate glass matrices were also studied as a reference inorganic host system. The obtained results demonstrate that polymer matrices provide a flexible platform for tailoring defect states and luminescence behavior of perovskite-based materials, which is essential for the development of stable hybrid photonic and scintillation devices.

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VITREORETINAL TAMPONADES AS OCULAR MATERIALS: FROM SILICONE OILS TO HYDROGELS

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Intraocular tamponades are essential materials used to stabilize the retina following vitreoretinal surgery, where long-term performance depends on interfacial behavior and

mechanical stability within a confined physiological environment. Silicone oils based on polydimethylsiloxane remain the most widely used tamponade agents; however, their functionality is frequently limited by shear-induced emulsification leading to droplet formation. In this context, silicone oil tamponades behave as confined multiphase systems in which composition, molecular architecture, and amphiphilic species govern interfacial rheology and droplet stability.

While emulsification is traditionally described as oil-in-water droplet formation, recent in vivo observations indicate that water-in-oil microstructures may also arise within the oil phase during prolonged intraocular residence. This expanded view emphasizes the role of interfacial viscoelasticity and local shear conditions rather than bulk viscosity alone. Strategies beyond simple viscosity adjustment, including incorporation of high-molecular-weight fractions, therefore aim to enhance interfacial viscoelasticity and improve resistance to emulsification.

Beyond incremental modification of silicone oil formulations, emerging hydrogel-based vitreous substitutes offer new material design opportunities with tunable viscoelasticity and potentially reduced susceptibility to emulsification. Hyaluronic-acid-based in situ crosslinked systems represent promising injectable materials capable of forming stable networks directly within the vitreous cavity. Integrating interfacial physics, polymer chemistry, and process-level considerations provides a framework for the design of next-generation ocular materials with improved long-term intraocular stability.

SCIENTIFIC AND TECHNOLOGICAL CHALLENGES IN THE FIELD OF ANTI-CORROSION AGENTS

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The lecture deals with the challenges facing both academia and industry in the field of anti-corrosion protection of iron and steel materials. These challenges are caused by several facts. First, it is true that alloyed metals are becoming increasingly expensive, and their problems are also the ethics of mining and geopolitical availability. Currently, so-called carbon steel is already massively used, which is associated with the development of advanced surface treatments and coatings that would replace expensive alloying throughout the entire volume of the material. However, organic coatings open up another big topic, which is the so-called biocorrosion caused by microorganisms.

Among the greatest current challenges and problems in the field of research and application of inorganic and organic anti-corrosion compounds is the growing pressure on environmental sustainability, regulation and limitation of toxic elements. Traditional effective compounds containing, for example, Cr^{6+}, Ba^{2+}, Sr^{2+}, Zn^{2+} ions are gradually being limited due to toxicity and environmental burden. As a result, there is a need to develop alternatives that provide comparable performance. The top challenge is the development of a new generation of so-called "smart" anti-corrosion systems with controlled release of inhibitors and nano pigments that improve the barrier effect. However, these bring challenges regarding dispersibility, compatibility with the binder and safety of nanoparticles, etc.

And since anti-corrosion compounds are also used in heat transfer fluids, rust removers and metalworking fluids, this also opens up the field of development of new formulations, where these formulations must now meet demanding hygienic and ecological requirements.

Another challenge is associated with the transfer from laboratories to practice. Long-term outdoor tests often do not correspond to laboratory accelerated tests. This makes development difficult, because many promising inhibitors fail in practical use.

JOINING HIGH-ENTROPY CERAMICS WITH HIGH-ENTROPY ALLOYS FORMED BY THE SAME REFRACTORY METALS

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High-entropy ceramics based on carbides (HEC) and borides (HEB) of refractory metals represent a group of ultra-high-temperature ceramic materials (UHTC), which typically exhibit very high hardness, strength, and fracture resistance, even at very high temperatures. Although individual types of HEC and HEB are still under investigation and their potential is being tested, methods for their joining are also being investigated. The joining process itself is complex issue, especially for UHTC. The joints studied in similar cases are mostly based on direct diffusion bonding, the use of in situ composites (e.g. with MAX phases in a refractory metal matrix), brazing, and related approaches.

Our work focused on the use of high-entropy alloys (HEA) based on five-component equimolar alloys of the same high-melting metals used for the preparation of HEC and HEB. High-entropy carbides based on (Hf-Zr-Ti-Ta-Nb)C and (Mo-Nb-Ta-V-W)C were prepared by solid-state synthesis from a powder mixture of the individual metal carbides. High-entropy borides (HEB) with the composition (Hf-Zr-Ti-Ta-Nb)B_2 and (Mo-Nb-Ta-V-W)B_2 were prepared by boron/carbothermic reduction of a mixture of the individual metal oxides. The materials were produced by powder sintering using Field Assisted Sintering Technology (FAST) or Spark Plasma Sintering (SPS). The HEAs were prepared either by

melting in an electron furnace followed by rolling with intermediate annealing to a final thickness of 100 μm, or by mechanical alloying and powder sintering by SPS; the joining interlayers were prepared by electric discharge machining and polishing. The joining process required optimisation of temperature, time regime, and pressure, as well as modification of the HEA microstructure to control the formation of secondary phases in the alloy due to diffusion through the HEC–HEA interface, using this process to slow diffusion or to enable strengthening of the HEA.

Detailed microstructural and phase analysis, performed by XRD of the produced materials and compounds, accompanied by detailed microstructural observation using scanning electron microscopy with local and area EDS analysis, showed significant changes at the HEC–HEA interface. However, from a microstructural integrity perspective, no defects such as cracks or non-bonding between HEA and HEC and/or HEB were observed that would affect fracture resistance. The prepared joints exhibited properties corresponding to those of the joined base materials or even better, including at temperatures above 1400°C.

MATERIALS AND PROCESS ENGINEERING

POSTERS

PREPARATION AND CHARACTERISATION OF Si_3N_4 CAPPING LAYER

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Phase change materials represent a group of chalcogenide alloys with exceptional properties. By adding heat, it is possible to switch rapidly and reversibly between amorphous and crystalline states. The change occurs within nanoseconds. These states have a high optical and electrical contrast because the phase change results in a sharp change in electrical resistivity and reflectivity. The differences between these states are exploited in non-volatile storage media where they form a recording layer or various photonic applications. The properties can be change by changing the composition of the alloy itself or by doping with additional elements. These materials are most often applied in the form of thin films with thicknesses ranging from nanometer to micrometer units.
Phase change materials films still face some challenges and have some shortcomings. These include phase stability, oxidation, reaction with moisture or mechanical damage. In addition to doping the elements, these undesirable effects can be combated with a capping layer. Silicon-based compounds such as SiN_x or SiO_2 seem to be an interesting choice. Si_3N_4 has a high dielectric constant, good thermal shock resistance, strength and high chemical stability. In the spectral range of 300–1200 nm, it achieves high transmittance.
Si_3N_4 layers were prepared by magnetron sputtering and subsequently characterized by spectroscopic ellipsometry, infrared spectroscopy, scanning electron microscopy and atomic force microscopy.

INVESTIGATION OF DEGRADATION OF TUNGSTEN-BASED MATERIALS FOR FUSION DEVICES USING THERMAL LOAD TESTING

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Plasma-facing components (PFCs) in fusion devices are exposed to extreme transient thermal loads. High melting temperature, excellent thermal conductivity, and resistance to sputtering and neutron-induced activation are key parameters for the PFC material selection. Tungsten and tungsten-based composites represent leading candidates for such applications. In this work, bulk tungsten and tungsten-copper composite materials

produced by various manufacturing processes were tested using an electron beam to simulate high thermal loads.
Thermal loading experiments were conducted using an electron beam facility, applying short heat pulses (~1 s) with power densities ranging from 10 to 40 $MW \cdot m^{-2}$, simulating plasma-induced transient events. Temperature evolution was monitored using embedded thermocouples and pyrometer and compared with theoretical thermal model.
The surfaces of the tested samples after thermal loading were characterized using scanning electron microscopy and profilometry. In most of the tested samples, a dense network of intergranular cracks was observed on the surface of tungsten and tungsten-copper composite in the loaded area. Inspection of a cross-section revealed well-developed cracks propagating in an intergranular manner only when exposed to the highest thermal load. Microstructural changes in terms of recrystallization of the material were observed at power densities above 30 $MW \cdot m^{-2}$. These results provide insight into the thermal stability and degradation mechanisms of tungsten-based materials exposed to thermal loads expected in experimental fusion devices.

RHEOLOGICAL BEHAVIOUR, STABILITY, AND MINERALOGICAL EVOLUTION OF RED GYPSUM AND FLUIDIZED BED FLY ASH WATER GROUTS FOR SUSTAINABLE GEOTECHNICAL APPLICATIONS

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The sustainable utilization of industrial byproducts is a key strategy for reducing environmental impact and promoting circular economy principles. This study explores the use of two byproducts – red gypsum (RG) and fluidized bed fly ash (FBFA) – as sustainable material for geotechnical applications. Utilizing these materials reduces reliance on primary raw materials, thereby lowering the ecological footprint of construction and remediation activities. The research focuses on three critical aspects: **(i)** rheological characterization, **(ii)** grouts stability analysis, and **(iii)** hydration analysis by in situ X-ray diffraction (XRD) for real time evaluation of hydration and Scanning Electron Microscopy (SEM) for morphology analysis after hydration. By integrating these methods, the study provides a comprehensive understanding of the performance and durability of these materials under realistic conditions of recultivation and throughout aging after placement. Preliminary results indicate a positive effect of fly ash on the rheology of red gypsum suspensions and confirm the crystallization of ettringite during hydration, which supports structural stability. The findings contribute to the development of environmentally responsible formulations that support sustainable infrastructure and land rehabilitation.

This study was conducted in collaboration with PRECHEZA a.s.

APPLICABILITY OF THE R3 TEST AND THE CHAPELLE TEST FOR DETERMINING THE POZZOLANIC ACTIVITY OF OVERBURDEN CLAYS

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Overburden clays are fine-grained, highly plastic sediments formed by weathering of primary minerals and rocks, whose chemical and mineralogical composition is highly variable. They often represent a by-product or waste material generated during the extraction of primary raw materials. Although these materials usually remain unused, their properties suggest that they could become an important secondary source for civil engineering in the future.
The aim of this study was to verify the suitability of the R3 test method according to ASTM C1897 for determining and evaluating the pozzolanic activity of calcined overburden clays. This suitability was evaluated by comparing the results of the R3 test with the commonly used Chapelle test (according to the NF P18-513 standard). Compared to the Chapelle test, the R3 test offers significant simplicity, lower requirements for laboratory equipment, and the ability to proceed autonomously without the need for continuous supervision.
The experimental part is based on monitoring changes in the bound water content in a mixture of calcined clay, calcium hydroxide and calcium sulfate during a seven-day reaction at 40 °C. The water content is determined as the mass difference before and after heating at 350 °C. The Chapelle test was carried out simultaneously as a reference method. The results provide an overview of the pozzolanic activity of various types of overburden clays and of the potential of the R3 test as an alternative, efficient analytical method for evaluating the pozzolanic activity.
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REGENERATION OF CELLULOSE FROM TEXTILE WASTE

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Chemical recycling of blended textile waste is a cornerstone of the transition toward a circular economy. This research focuses on the sustainable management of cellulose-based waste using imidazolium-based ionic liquids (ILs): 1-ethyl-3-methylimidazolium acetate (EMIMAc), 1-allyl-3-methylimidazolium chloride (AMIMCl), and 1-ethyl-3-methylimidazolium chloride (EMIMCl). Industrial cord viscose, characterized by high crystallinity and exceptional chain length, was selected as a model material to test the limits of the dissolution process. The study assumes that procedures successful for such resistant cellulose are applicable to a wide spectrum of common textile waste.

The experimental work investigates the preparation of viscous cellulose solutions and their subsequent transformation into new structural arrangements via antisolvent precipitation. Depending on process parameters, the regenerated cellulose was formed into either transparent films or fibrous textures resembling cotton wool. While these ILs effectively disrupted the dense hydrogen bond network of the cord viscose, Thermal Gravimetric Analysis (TGA) of the products revealed a critical challenge: high residual masses (88.9–94.3% at 300 °C). These findings, supported by FTIR spectroscopy, indicate significant entrapment of the ionic liquid within the regenerated polymer matrix.

A key component of this study is the evaluation of solvent recovery efficiency. Using vacuum regeneration in a rotary evaporator system, the ILs were stripped of antisolvent residues for potential reuse. However, the observed solvent retention in the regenerated cellulose presents a major economic and technological hurdle. The results provide a necessary basis for discussing the feasibility of material recovery from difficult-to-recycle textiles, balancing the superior performance of ionic liquids against the imperative of solvent recovery and overall process costs.

INFLUENCE OF SURFACE DEGRADATION ON THE SORPTION PROPERTIES OF MG–NI POWDER MATERIALS

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The study is aimed to investigate the influence of surface degradation on the hydrogen sorption properties of Mg–Ni-based powder materials and how exposure to air and gaseous hydrogen condition at elevated temperatures affects these properties.
The experimental material consisted of Mg–Ni-based powder, whose chemical composition was confirmed by SEM–EDS analysis. Thermal exposures were subsequently performed in the air at 200 °C and 350 °C, with parallel treatments conducted under identical conditions in a gaseous H_2 atmosphere. Changes in hydrogen sorption behavior following each exposure were assessed using differential scanning calorimetry (DSC).
The results showed that at lower exposure temperatures and shorter durations, surface oxidation was limited and did not fully suppress hydrogen sorption. Although a decrease in sorption capacity was observed, the material retained partial functionality. In contrast, higher temperatures caused pronounced surface degradation, likely due to the formation of stable oxide layers, leading to an almost complete loss of sorption capability.
The findings highlight the critical importance of controlling exposure and handling conditions to preserve the functional properties of Mg–Ni materials intended for hydrogen storage applications, confirming their high sensitivity to surface oxidation processes.

THE EFFECT OF SIZE AND CONCENTRATION OF GRAPHENE NANOPARTICLES ON IMPROVEMENT OF THERMOPHYSICAL PROPERTIES OF NANOFLUIDS.

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For efficient heat transfer in heat exchangers, the heat transfer fluid must not only have sufficiently high thermal conductivity but also low viscosity to prevent an increase in pump power due to high pressure loss. Water is the traditional fluid used for efficient heat transfer. Thermophysical properties of water can be improved by adding suspended nanoparticles of solids with high thermal conductivity. However, when replacing traditional water with these modern nanofluids, it is necessary to monitor the increases in both thermal conductivity and viscosity. Improved heat transfer can only be expected if the relative increase in viscosity does not exceed four times the increase in thermal conductivity. Nanofluids are considered stable enough for use in heat exchangers if any deposits can easily be redispersed, meaning the nanoparticles remain suspended during flow in the exchanger.
This paper presents a case study of nanofluids containing graphene particles of three different sizes (2 nm, 6–8 nm, and 11–15 nm) and various concentrations in distilled water. Tannin was added as a dispersant at a concentration of 50% by weight of graphene. The addition of small graphene nanoparticles (2 nm) was shown to lead to stable nanofluids, which, however, do not exhibit an increase in thermal conductivity. In contrast, the addition of larger graphene nanoparticles (6–8 nm and 11–15 nm) significantly increases in thermal conductivity compared to distilled water (by 10–20%), even at lower concentrations. Since the increase in viscosity (by 10–30%) does not exceed the threshold level of a fourfold increase in thermal conductivity, these nanofluids will be tested in a pilot heat exchanger.

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STUDY OF CARBONATION OF THE THREE-COMPONENT HYDRAULIC BINDER 3C AS AFFECTED BY DIFFERENT CALCINATION METHODS

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This study investigates the carbonation of a novel hydraulic binder 3C, composed of three components—calcined clay, anhydrite II, and lime. For the experimental program, a series

of binders was prepared by calcination of kaolinitic clay, gypsum, and limestone. The raw materials were fired both separately and together in a static kiln and a rotary kiln. The firing procedures were designed so that, despite different calcination approaches, the final chemical composition of all prepared 3C binders remained comparable. The carbonation depth was determined on hardened paste cubes with dimensions of 20 mm prepared with a water-to-binder ratio of w = 0.5–0.6. Accelerated carbonation conditions were applied, where the specimens were exposed in a climatic chamber to an atmosphere containing 3% CO_2 at 30 °C and 65% relative humidity. The carbonation progress was evaluated on cross-sections of the cubes after 7, 14, and 28 days using the phenolphthalein test. In addition, compressive strength, phase composition, and pore structure were determined. The phenolphthalein test results indicated a significant decrease in binder pH after a relatively short exposure to carbon dioxide. Carbonation also adversely affected the mechanical properties, leading to a substantial reduction in compressive strength. Phase analysis suggested the decomposition of the main crystalline phase, ettringite, and the formation of gypsum phases. Measurements of the pore structure further revealed an increase in the overall porosity of the carbonated specimens.

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CZECH NEUTRON ASSOCIATION

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The Czech Neutron Association is a professional society bringing together scientists, students, and other specialists who make use of neutron radiation in their work. The mission of the association is to support the development of research in this field at both the national and international level, to connect the expert community, and to actively advocate for its interests.
The association strives to strengthen the position of neutron research in the Czech Republic not only by supporting scientific collaboration, but also by engaging with European and global infrastructures. It serves as an open platform for sharing information, coordinating activities, and fostering strategic dialogue among research institutions, public authorities, and the wider public.

Our goals are to:

- connect the community of Czech neutron users across disciplines and institutions
- promote research using neutron radiation across the full spectrum of scientific fields

- facilitate communication between the expert community, academic institutions, public authorities, and the general public
- represent the Czech Republic in international neutron structures, institutions, and thematic networks

PELETY Z OVČÍ VLNY – POMOCNÝ PŮDNÍ PROSTŘEDEK

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Domácí chovatelé pociťují významné problémy s odbytem ovčí vlny. Trh oděvních aplikací je zaplaven poměrně levnou vlnu z dovozu. Ovce se však musí průběžné stříhat; vlna se tak pro chovatele stává vlastně odpadem. Na ovčí vlnu je ale možno pohlížet jako na přírodní surovinou, která je biologicky rozložitelným materiálem s širším možným využitím. Jednou z možných aplikací je použití vlny jako pomocného půdního prostředku podporující růst pěstovaných rostlin, případně příznivě ovlivňující strukturu a další vlastnosti půdy. Pro tyto účely je vhodné vlnu zpracovat do formy válcovitých pelet. Alternativou je kompostování vlny. Obecně může vlna působit jako prostředek pomalu uvolňující dusíkaté živiny; kompostovanou ovčí vlnu lze použít jako příměs pěstebních substrátů a náhradu rašeliny. Tento příspěvek uvádí výsledky vybrané fyzikálně-chemické charakterizace pelet z vlny pocházející z českého chovu. Konkrétně

- sušicí křivky pelet i vlny,
- stabilita/rozpad pelet ve vodném prostředí,
- nasákavost pelet v atmosféře o různé vlhkosti (s řízeným obsahem vody ve vzduchu);
- mechanická pevnost pelet v tlaku;
- termogravimetrická analýza surové vlny;
- infračervená spektroskopie surové vlny;
- skenovací elektronová mikroskopie vláknité struktury pelet.

Tyto charakteristiky mají význam pro přípravu, skladování či přepravu pelet a poskytují základní informace o jejich funkčním složení a chování při aplikaci do půdy a následné závlaze.

Tato práce je podpořena projektem TAČR SQ01020087, Využití odpadní surové ovčí vlny v zahradnické produkci.

CHARACTERISATION AND THERMAL PLASMA PROCESSING OF TOMATO BIO–POLYMER WASTE

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Agro-industrial residues increasingly occur as heterogeneous mixtures of lignocellulosic biomass and synthetic polymers originating from cultivation and processing chains. In tomato production, post-harvest residues are largely composed of dried, crushed stems mixed with polypropylene twines used for plant support. These bio–polymer blends are difficult to recycle mechanically or chemically due to their mutual dispersion and compositional variability. Moreover, agricultural residues can exhibit significant differences in inorganic content, as ash composition reflects soil properties, geographical location and cultivation conditions, complicating standardised treatment strategies. This work investigates thermal plasma processing as a flexible and sustainable approach for the treatment and valorisation of crushed tomato waste in a laboratory-scale thermal plasma reactor. A substantial fraction of the organic matter is converted into synthesis gas rich in hydrogen (H_2) and carbon monoxide (CO), which can serve as a secondary energy carrier or chemical feedstock after appropriate conditioning. The study focuses primarily on comprehensive characterisation of input materials and process products in order to establish reliable material, elemental and energy balance frameworks. Proximate and ultimate analyses are complemented by detailed ash characterisation to assess the influence of inorganic constituents on process behaviour. Results are interpreted in the context of previous plasma experiments with bio-waste (specifically coffee grounds), enabling direct comparison of selected material and process characteristics. Particular attention is devoted to the solid output fraction, consisting of mineral ash and plasma-generated carbonaceous particles. The morphology, structure and surface properties of the carbon-rich fraction are evaluated with respect to potential material applications, such as functional carbon materials. Environmental aspects are considered in terms of chemical stability and basic safety assessment of both feedstock and solid residues. The presented work contributes to the development of a robust and reproducible plasma-based platform for processing compositionally complex agricultural bio–polymer waste within circular carbon management strategies.

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SHAPE MEMORY EFFECT OF ATOMIZED FRACTIONS OF NI-TI-CU-ZR-HF ALLOY

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In this study, the influence of the atomization process and powder size fraction on the martensitic transformation temperature of a Ni–Ti–Cu–Zr–Hf alloy was investigated. The chemical composition of the as-cast alloy was verified by XRF prior to atomization, followed by separation into individual powder fractions (0–63 µm, 63–80 µm, 80–150 µm, 150–500 µm, 500–1000 µm and >1000 µm). The fractions were characterized using laser diffraction and µCT to statistically describe particle size distribution and internal morphology. Phase composition and transformation behavior were analyzed by X-ray diffraction and DSC, while microstructural features and chemical homogeneity were examined by SEM-EDS and WDS. The powders exhibited an inhomogeneous dendrite-based microstructure depending on particle size. The shape memory effect was confirmed not only in the as-cast state but also in the mixed powder fractions, with the martensite start temperature (Ms) determined at 220 °C. This study confirmed the preservation of the high-temperature shape memory effect in the atomized powders, enabling the application of advanced processing technologies and further development of these materials for practical use.

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CORROSION BEHAVIOUR OF PLASMA-NITRIDED Y1860 S7 PRESTRESSING STEEL FOR BRIDGE STRUCTURES

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Recent collapses of several bridges caused by corrosion of prestressing reinforcement have intensified research efforts aimed at improving the corrosion protection of such reinforcement, particularly through surface coatings. Nitriding is generally known to enhance corrosion resistance; however, during the initial stage of the process, the forming nitride layers with variable stoichiometric composition act as a barrier limiting further nitrogen diffusion into the bulk of the material. This retardation effect of the surface layer, typically composed of Fe_2N and Fe_4N phases, necessitates prolonged exposure of the steel to elevated temperatures in order to achieve sufficient nitriding throughout the material volume. Such extended thermal exposure may negatively affect the mechanical properties of the steel due to tempering effects. Conventional steel nitriding, commonly performed using atomic nitrogen generated by the thermal decomposition of ammonia, ion nitriding in glow-discharge plasma where an electrical discharge accelerates nitrogen ions toward the steel surface, or nitriding in molten salt baths (an environmentally problematic method), typically requires reaction times on the order of several hours. In contrast, nitriding in water-stabilized plasma, characterized by a high concentration of N^+ and NO^+ ions, enables a significant reduction in the reaction time. However, the presence of oxygen ions in the plasma also promotes the formation of oxide films on the surface and reduces the content of the desired nitride phases. This study compares the results of nitriding of Y1860 S7 prestressing steel performed using three different approaches: conventional nitriding in an atmosphere of thermally decomposed ammonia at 1250 °C, reaction with molecular nitrogen during prolonged heating of the steel at 1250 °C, and treatment of pre-oxidized steel in water-stabilized plasma generated in a WSP H-160 plasmatron. The surface-treated prestressing steel samples were subsequently subjected to corrosion testing during exposure to chloride solutions. Furthermore, the bond strength between the coated prestressing reinforcement and concrete was evaluated according to ČSN 73 1333. The results indicate that nitriding increases the bond strength between the reinforcement and concrete by approximately 5–7%.

REACTION OF CALCIUM FLUORIDE WITH GROUP 4 METALS

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Calcium fluoride, apart from its use as a raw material source for the production of fluorine and hydrofluoric acid and in the steel industry as a melting agent for reducing the melting temperature of slag, has recently become particularly important in optics and laser technology, thanks to its exceptional permeability for ultraviolet (UV) and infrared (IR) radiation. Its processing for these purposes requires high temperatures, or its use in a molten state. Due to its high reactivity at high temperatures, including reaction with oxygen or water vapour (often mistakenly referred to as oxidation in the literature), the choice of suitable auxiliary structural materials, stable above the melting temperature of 1693 K, is very limited. The most common are graphite, platinum or Pt-Rh alloys. Data on the use of ceramic, especially oxide, materials are not reliable, due to the previously proven ability of calcium fluoride to form eutectics with lower melting points. This paper presents the results of X-ray structural and microscopic analysis of the interface after reaction of fused CaF_2 with powdered or large-scale substrates of high-melting metals of 4th group. The interaction of calcium fluoride with titanium, zirconium or hafnium occurs mainly in the case of their slightly oxidized surface, the quantitative analysis of which is always below the level of detection by available methods of X-ray analysis or by the LECO method, or their oxidation in a non-inert environment occurs before the reaction of calcium fluoride with a temperature above about 800°C is achieved.

CALCIUM FLUORIDE COATINGS AGAINST HYDROGEN FLUORIDE CORROSION

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Surface protection of metallic materials, especially steels, against the action of hydrofluoric acid or hydrogen fluoride gas at high temperatures is possible only by ceramic coatings made of insoluble compounds that are temperature-stable in an oxidizing medium up to temperatures close to the melting points of selected metal substrates. The paper describes the preparation of calcium fluoride CaF_2 coatings by the method of surface melting in a boron nitride environment and compares with the method of thermal plasma spraying

using the WSP-H 500 water-stabilized plasma generator. CaF_2 coatings have been subjected to corrosion tests in aqueous solutions of hydrofluoric acid. A critical problem remains the irreversible and content-different presence of calcium oxide CaO in the commercial CaF_2 used, or its formation by reactions in water-stabilized plasma. The thermodynamic evaluation of the course of the melting processes favors the reaction of CaF_2 to CaO conversion by H_2O over the reaction with oxygen at temperatures above 800°C. CaF_2 coatings with a maximum content of up to 10 % CaO inhibit the corrosion of metal substrates with hydrogen fluoride by opposing CaF_2 regeneration reactions with gradual secondary sealing of pores and cracks in the coating. Along with this, the corrosion of surface-oxidized steel substrates is slowed down by the secondary formation of poorly soluble iron fluorides, which act as a temporary passivation film at the ceram-metal interface.

ADDITIVE MANUFACTURING OF NITINOL BY DIRECTED ENERGY DEPOSITION USING POWDER AND WIRE FEEDSTOCKS

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Nickel–titanium alloys (NiTi), commonly referred to as Nitinol, belong to a group of shape memory alloys characterized by unique functional properties such as the shape memory effect and superelasticity. These properties arise from a reversible martensitic transformation and make NiTi highly attractive for applications in biomedical devices, actuators, and advanced engineering components. However, conventional manufacturing of NiTi is technologically demanding due to its high chemical reactivity, sensitivity to composition variations, and difficulties in machining.
Additive manufacturing technologies provide new possibilities for producing complex NiTi components. In particular, the Directed Energy Deposition (DED) process enables the fabrication of components with complex geometries, often with a minimal need for subsequent machining operations. In laser-based DED, the feedstock material can be delivered either in the form of powder or wire, both of which are melted by a focused laser beam and deposited layer by layer.
The aim of this work is to compare the properties of nitinol prepared by directed energy deposition using powder and wire feedstock. The materials were evaluated both in the as-built condition and after heat treatment consisting of solution annealing followed by aging. The study focused on the characterization of microstructure and phase

composition. Mechanical properties were evaluated by tensile testing, and superelastic behavior was assessed using cyclic superelastic tests.

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COMPLEX CONCENTRATED ALLOYS EXHIBITING HIGH-TEMPERATURE MARTENSITIC TRANSFORMATION

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Materials science is constantly searching for new alloys with unique properties that can be used in high-tech applications, from aerospace to medical devices. One exciting area of research focuses on complex concentrated alloys (CCAs), a special class of materials that mix multiple elements to achieve remarkable properties. This study explores the behavior of a specific group of CCAs based on Cu-Ni-Ti-Zr-Hf. These alloys can undergo a martensitic transformation, a reversible change in their internal structure that enables them to "remember" and return to their original shape after deformation. This property is highly desirable for applications requiring materials that can withstand extreme conditions while maintaining their functionality. By adjusting the amounts of Zr and Hf, as well as studying grain size and microscopic structures within these alloys, researchers aim to fine-tune their transformation temperatures and mechanical properties. A key goal is to compare these alloys with traditional NiTi alloy to determine their potential for high-temperature applications.
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APPROACHING THE OPTICAL BANDGAP LIMIT: DONOR–ACCEPTOR ENGINEERING AND Π-CONJUGATION EXTENSION TOWARD NIR FLUORESCENCE

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Near-infrared (NIR) fluorescent materials are highly attractive for applications in bioimaging, optoelectronics and security technologies. Achieving efficient NIR emission fundamentally requires a significant reduction of the optical bandgap, while maintaining sufficient oscillator strength and radiative decay rates.

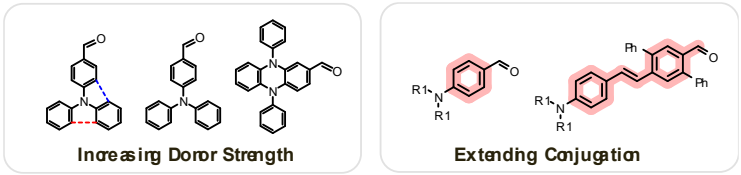

Figure 1. Strategies to reach NIR fluorescence.

The first strategy is based on strengthening the intramolecular charge transfer (ICT) through incorporation of strong electron-donating and electron-accepting units. In the stilbene series, increasing donor strength enables systematic emission tuning across a broad spectral window, with maxima spanning from 511 to 787 nm in dichloromethane. Using the *N,N'*-diphenyl-dihydrophenazine (DPPZ) donor, introduction of electron-withdrawing substituents significantly stabilizes the LUMO level and narrows the optical bandgap down to approximately 0.93 eV. This electronic modulation is reflected in pronounced bathochromic shifts of emission, with selected derivatives exhibiting fluorescence ranging from 593 to 955 nm (DCM).

The second strategy focuses on π-conjugation extension. In our systems, the donor (diphenylamine, 9/3-phenylcarbazole or DPPZ) is connected to the acceptor through a stilbene spacer, effectively extending the π-system. For comparison, we prepared structurally analogous derivatives featuring direct donor–acceptor linkage without the additional conjugated bridge. The extended stilbene architecture consistently exhibits narrower bandgaps and more pronounced bathochromic shifts compared to the directly linked analogues. The authors express their gratitude for financial support from the Czech Science Foundation, grant No. 24-10479S.

CENTRAL–SHIELDING GAS FLOW SEPARATION SIMULATION IN MICROWAVE PLASMA TORCHES

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Microwave plasma torches operating at atmospheric pressure are increasingly used for high-temperature chemical processes, materials synthesis, and gas conversion due to their electrode-free operation and high energy density. For many mentioned uses, maintaining a separated central plasma column and annular shielding gas flow at high flow rates remains a significant challenge, particularly due to shear-layer instabilities and flow asymmetry.
In this work, we investigate torch design optimization aimed at separating central and shielding gas flow in a microwave plasma torch operating at 2.45 GHz and 6 kW. A coaxial gas injection swirl-inducing geometry is simulated using CFD simulations performed in ANSYS Fluent software with various conditions in which the process gas forms a central plasma stream while an annular shielding flow protects reactor walls and stabilizes the discharge. The influence of flow rate ratios and inlet geometry was studied.
Flow separation influences mixing behaviour and residence time of reactive species within the plasma core, optimizing central flow for gas decomposition and synthesis reactions. Appropriate shielding flow significantly reduces radial plasma expansion and prevents plasma attachment to reactor walls. These findings highlight the importance of simulation-based hydrodynamic design of microwave plasma reactors for improving plasma stability in high-throughput plasma processing systems.

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Citations:
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BIOTECHNOLOGY AND BIOREFINERY

LECTURES

WASTE-BASED BIOREFINERIES: UNLOCKING THE POTENTIAL OF RESIDUAL BIOMASS FOR A SUSTAINABLE CIRCULAR ECONOMY

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Biorefineries are at the heart of the modern bioeconomy, supporting substitution of fossil resources with sustainable, bio-based feedstocks. They integrate a variety of biological, chemical, and physical processes to convert biomass into a wide range of valuable products—from platform chemicals and bioplastics to energy. Currently, over one thousand biorefineries exist worldwide, differing in terms of feedstock (e.g., crops, waste, manure) and target products. While first generation biorefineries are mainly supplied by food crops, advanced facilities increasingly rely on residues and waste streams.
The harnessing of waste streams therefore represents one of the most resource-efficient routes, providing both ecological and economic advantages. Data demonstrates a vast annual volume of organic residues with diverse components, much of which remains underused. Biorefineries realise these potentials and support cascading use of biomass: from high-value chemicals such as lycopene recovered from tomato or pepper residues to the valorisation of pig manure, where anaerobic fermentation allows the recovery of nutrients and energy. Even when the production of high-value products is not feasible, energy recovery through heat generation remains a viable option.
The increasing application of anaerobic fermentation processes enables the production of new platform chemicals, such as volatile fatty acids (VFAs), from wastewater streams. Such innovations broaden the range of target products and create new value chains. Real-world examples illustrate the diversity and innovation potential of modern biorefineries.
In conclusion, biorefineries play a key role in the transition towards a sustainable circular economy. The consistent utilisation of waste and residual streams offers the greatest leverage: ecologically, economically, and socially.

RESILIENCE OF ACTIVATED SLUDGE TO WASTEWATER FROM PARTIAL OXIDATION PROCESS: IMPACTS, INHIBITION AND ADAPTATION

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The partial oxidation unit for oil residues represents a key technology producing hydrogen at the ORLEN Unipetrol's site. One of its by-products is so-called soot water, a wastewater stream characterised by high concentrations of ammonia, sulphides, cyanides, thiocyanates, heavy metals, and other critical pollutants from previous processing. Currently, this wastewater is partially detoxified and discharged to the New Ash Landfill,

whose capacity will be exhausted soon. These circumstances highlight the necessity to integrate the soot water into the wastewater treatment process.
The research focuses on assessing the impact of soot water and by-products of its partial detoxification on the operation of a biological wastewater treatment plant and on the stability of its activated sludge using a laboratory-scale model.
Even at increasing concentrations of thiocyanate up to 100 mg/L, no conclusive inhibitory effect on the microbial activity of the activated sludge was observed. During the experiment, however, cyanide ions appeared in the biological reactor at a concentration of 3 mg/L, resulting in measurable inhibition of nitrification. At the same time, the microbial community exhibited adaptive changes in species composition, enabling it to deal better with the increased thiocyanate concentrations.
The results provide important insights into the behaviour of the detoxified soot water during biological treatment and support future decision-making for handling this complex wastewater stream.

FEATHERS, GRAINS, AND MICROBES: NEW STRATEGIES FOR CONCRETE WASTE RECYCLING

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In 2024, total waste production in the Czech Republic exceeded 40 million tons according to the Czech Statistical Office, representing a 6 % increase compared to the previous year. The largest share (57.2 %) consisted of mineral waste, which includes construction and demolition materials. Up to 40 % of this waste consists of a fine fraction below 1 mm. Due to its dustiness and high specific surface area, it has no further practical use, and current legislation requires its landfilling. However, this fraction can be recycled through microbially induced calcite precipitation (MICP), in which the precipitated crystals act as a binder for fine particles. This process consolidates the material and forms a biocomposite that meets the requirements for selected construction applications, such as pavement sub-base layers. For the technology to be applied on a larger scale, it is crucial to reduce production costs, up to 60% of which are associated with the cultivation medium. Therefore, we investigated food-industry waste as a nutrient source for bacteria capable of MICP. Chicken feathers represent a rich source of protein, and we optimized their hydrolysis based on the growth performance of *Sporosarcina pasteurii* DSM 33 and *Sutcliffiella cohnii* DSM 6307. These strains employ distinct biochemical pathways leading to MICP; notably, the organic acid-oxidizing *S. cohnii* exhibits a significantly lower carbon footprint than the ureolytic *S. pasteurii*. We also focused on brewery by-products, such as spent grains and yeast biomass. Using alternative media, we produced biocomposite samples and analysed them using scanning electron microscopy, X-ray diffraction, thermogravimetric analysis, and mechanical testing. Biocomposites prepared with

alternative media displayed properties comparable to those obtained using commercial media. By reducing media costs by 80 %, this approach moves the technology closer to real-world application while simultaneously promoting the valorisation of various waste streams within a circular-economy framework.

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ENHANCING BIOREFINERY CONTROL AND OPERATION WITH A NEW TRAINING SIMULATOR

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Biorefineries convert biomass as a feedstock into a spectrum of bio-based value added products (food, chemicals, materials) and bioenergy (biofuels, power and/or heat) [1]. However, the development of operation and control strategies for complex biorefineries is not straightforward. In this contribution a new simulator shall be presented, utilisable for academic and industrial training.
The BioRefineryTrainer is the virtual image of a pilot plant in which renewable raw materials containing starch and proteins are converted into valuable products like bioethanol, baker's yeast or ethyl (S)-3-hydroxybutyrate (E3HB, kiwi flavour). The process comprises four interacting unit operations: (1) enzymatic hydrolysis of starch and protein rich raw materials, (2) cultivation of the yeast *Saccharomyces cerevisiae* and ethanol production (3) microfiltration to mimic cell recirculation and (4) rectification for ethanol recovery (Figure 1).

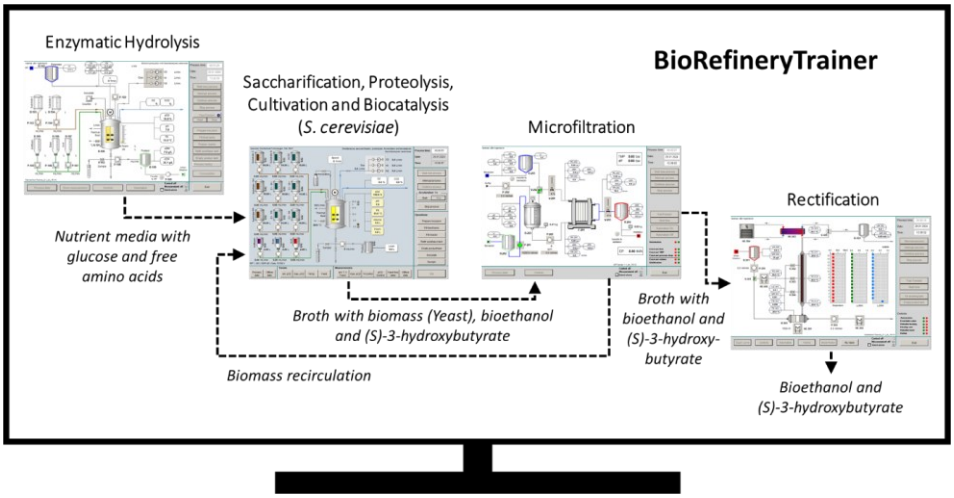

Figure 1: Structure of the BioRefineryTrainer

For the unit operations, independent simulators were created based on core models, describing the time courses (dynamics) of each unit operation. The core models of the simulators [2-5] are written in the C++-based simulation and modelling software C-eStIM [6] and were parameterised using experimental data from pilot plant processes. The C-eStIM -DLLs were implemented in the WinErs process control and simulation system [7]. WinErs allows for the easy implementation of PID-controllers and automation strategies as well as GUI development. Data from the biorefinery simulator can be viewed online in the form of graphs as well as monitored for subsequent analysis. This allows for the analysis of a wide range of process control strategies.

By using the BioRefineryTrainer, students and future plant operators can learn and train the operation of a biorefinery and the basics of control engineering, in an innovative hands-on and illustrative way.

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PRINCIPLE(S) OF ANTIMICROBIAL ACTIVITY OF *MONASCUS* PIGMENTS

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Fungi of the genus *Monascus* are known for producing secondary metabolites, primarily pigments, which are mainly used for coloring food. However, pigments also have various biological effects. There are a number of articles dealing with the antimicrobial activity of *Monascus* pigments. Unfortunately, in most cases, the authors of these articles used extracts from mycelium or fermented rice of unknown composition. Pigments are divided according to color into yellow, orange, and red. As the antimicrobial activity of orange pigments, rubropunctatin and monascorubrin, is very difficult to determine because these pigments are highly reactive and react with compounds containing a primary amino group, such as amino acids, at neutral or slightly acidic pH, the most reputable measurements therefore focus on yellow, ankaflavin and monascin, and red, rubropunctamine and monascorubramine, pigments. The minimum inhibitory concentration (MIC) of red pigments with bound amino acids varies depending on the type of amino acid and ranges from 4 to 128 µg/ml. Pigments with bound L/D-cysteine, L/D-phenylalanine, L/D-tyrosine, and L/D-aspartic acid have the highest activity against G+ bacteria. In addition, they can inhibit the germination of asexual fungal spores, such as conidia of the genus *Aspergillus*. It appears that pigments disrupt cell surfaces through various mechanisms, interfering with transport into and out of cells as well as cellular respiration.
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IN-SILICO STUDY TO ANALYZE HOTSPOT RESIDUES OF MONASCUS PIGMENTS BINDING WITH CLOSTRIDIUM BEIJERINCKII GERMINATION PROTEIN FOR ANTIMICROBIAL EFFECTS

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Monascus pigments are natural food-derived colorants that have attracted increasing scientific interest because of their additional functional properties, particularly their potential antimicrobial activity. Commonly associated with traditional Asian fermented foods, these pigments include compounds such as rubropunctatin, rubropunctamine, and monascuspilion. Previous studies suggest that these metabolites may inhibit Clostridium species through multiple mechanisms, including membrane destabilization and disruption of spore germination. However, the molecular basis of their anti-germination activity remains poorly understood.

In this study, we performed a comprehensive *in-silico* molecular modeling analysis to investigate the interactions of Monascus-derived pigments with AlphaFold2 modeled spore-germination protein from *Clostridium beijerinckii*. Molecular modelling simulations analysis were employed to characterize the binding behavior of the selected pigments. The results revealed favorable and stable binding modes, primarily mediated by ionic, hydrogen-bonding, and hydrophobic interactions involving the key residues GLU245, TYR275, and ARG286.

To further assess their antimicrobial lead potential, ADMET profiling was carried out for all investigated pigments. The compounds showed favourable physicochemical and pharmacokinetic properties, including adequate aqueous solubility, lipophilicity, human intestinal absorption, bioavailability, and acceptable clearance profiles. Toxicity predictions indicated moderate hepatotoxicity and a low likelihood of hERG inhibition, suggesting an overall acceptable safety profile. Overall, these findings highlight the potential of Monascus pigments as natural antibacterial candidates for food safety applications and possible future biomedical use.

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EFFECT OF NATURAL AND SYNTHETIC MATERIALS' SURFACE TOPOGRAPHY ON BACTERIAL CELL ADHESION

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Bacterial biofilms present a serious issue in both medicine and industry, as they increase microbial resistance to disinfectants and therapeutic agents. Considering the growing antibiotic resistance, it is desirable to develop alternative strategies to reduce bacterial adhesion without the use of chemical agents. One promising approach is to utilise specific surface structures inspired by natural materials that exhibit inherent antibacterial effects. This study evaluated the influence of the topography of selected natural and synthetic nanofibrous materials on the adhesion and biofilm formation of *Escherichia coli* and *Staphylococcus aureus*. The tested materials included snakeskin and rose petals, as well as electrospun polycaprolactone nanofibers with smooth and modified surfaces. In the initial phase, the dynamics of biofilm formation were studied to determine suitable time points for evaluating bacterial adhesion and growth. Surface topography was assessed using scanning electron microscopy (SEM), and antibacterial activity was evaluated quantitatively by determining CFU/cm². The results showed that only the sharp protrusions on the scales of snakeskin significantly reduced bacterial adhesion. These structures served as inspiration for the design of biomimetic synthetic fibres, whose effectiveness was further experimentally tested. However, the antibacterial activity of the synthetic nanomaterials was not conclusively demonstrated. Overall, the results demonstrate that specific natural surface topographies can markedly suppress bacterial attachment and provide new insights for the design of synthetic materials with inherent antimicrobial properties.

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SYNTHETICALLY PRIMED ADAPTATION OF BACTERIAL CATALYSTS TO NON-NATIVE RENEWABLE SUBSTRATES

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Efficient valorization of renewable lignocellulosic substrates - sugars and aromatics - remains critical for the development of viable bioprocesses. However, many industrial

microbes lack efficient pathways for pentose, oligosaccharide, or aromatic compound assimilation. To address this, rational metabolic engineering is often combined with adaptive laboratory evolution (ALE), though comprehensive, systems-level studies on the resulting adaptations are still limited.

Here, we present a systems biology-driven investigation into the synthetic adaptation of *Pseudomonas putida* to non-native sugar substrates. Previously engineered strains capable of utilizing D-xylose, D-cellobiose, and D-glucose served as starting point. Despite the introduction of heterologous pathways, substrate assimilation remained inefficient. Using a suite of complementary approaches - fluxomics, proteomics, genomics, enzyme and growth assays, reverse engineering, and an enhanced genome-scale metabolic model constrained by kinetic and proteomic data - we dissected the adaptation process in detail.

Our analyses reveal how rational engineering primed *P. putida* for effective laboratory evolution on xylose.[1] Moreover, we identified mutants with improved aerobic co-utilization of glucose and cellobiose, capable of overproducing pyruvate and downstream products.[2] In addition, bacteria endowed with xylose, cellobiose and xylobiose utilization capacity were arranged in a two-strain consortium with a new type of synthetic mutualistic relationship.[3] This work exemplifies the power of integrated multi-omics in elucidating and guiding microbial adaptation to synthetic metabolic modules. The resulting insights not only inform future engineering of *P. putida* cell factories but also contribute to our fundamental understanding of how bacteria adapt to utilize non-native renewable carbon sources.

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RATIONAL TRANSPORTER ENGINEERING OUTPERFORMS ADAPTIVE EVOLUTION FOR GLUCOSE UTILIZATION IN THERMOPHILIC *CALDIMONAS THERMODEPOLYMERANS*

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Efficient valorization of lignocellulosic hydrolysates requires microbial hosts capable of utilizing mixed sugars, including glucose. The thermophile *Caldimonas thermodepolymerans* is a promising platform for biodegradable bioplastics production

from lignocellulosic residues but exhibits negligible growth on glucose despite genomic and metabolic model predictions indicating a complete glucose catabolic network. This discrepancy suggests that glucose uptake rather than intracellular metabolism limits glucose utilization.
To overcome this limitation, we compared adaptive laboratory evolution (ALE) with rational engineering of a heterologous glucose transporter Glf from mesophilic bacterium *Zymomonas mobilis*. ALE enabled growth on glucose at 50 °C and revealed mutations mainly in global regulatory genes, indicating indirect physiological adaptation. In parallel, thermostable Glf variants were designed and expressed in *C. thermodepolymerans* to directly improve glucose transport at elevated temperature. Growth analysis at 50 °C showed that the rationally designed transporter conferred the strongest improvement in glucose utilization, supporting faster growth and higher biomass than ALE-derived strains. Thus, targeted stabilization of a single membrane protein provided a larger phenotypic benefit than genome-wide adaptive evolution. The optimized strain further demonstrated efficient glucose consumption and improved co-utilization of glucose with xylose and cellobiose, highlighting its relevance for lignocellulosic bioprocessing.
Overall, our results identify glucose transport as the key bottleneck in *C. thermodepolymerans* and show that rational protein engineering can surpass adaptive evolution in overcoming thermophilic transport limitations. Engineering thermostable sugar transporters therefore represents an effective strategy for developing robust high-temperature microbial cell factories for mixed-sugar bioconversion.

TRANSCRIPTOMIC RESPONSE OF *CLOSTRIDIUM BEIJERINCKII* NRRL B-598 TO LIGNOCELLULOSE-DERIVED INHIBITORS

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Microbial solvent production is a promising approach for the sustainable generation of biofuels and value-added chemicals. In solventogenic clostridia, this occurs via acetone–butanol–ethanol (ABE) fermentation. Lignocellulosic biomass is an attractive substrate for such bioprocesses; however, its pretreatment releases inhibitory compounds that can negatively affect microbial growth and solvent production. To investigate cellular responses, we examined global transcriptional changes in *Clostridium beijerinckii* NRRL B-598 exposed to selected lignocellulose-derived phenolic inhibitors and their detoxification products.
RNA-Seq datasets were generated for three conditions: control (no inhibitors), exposure to inhibitors, and exposure to detoxification products. For each condition, samples were collected at two time-points corresponding to the acidogenic and solventogenic phases, enabling a comparison of transcriptional responses before and after the metabolic shift. The resulting datasets were analyzed using comprehensive bioinformatics approaches to characterize genome-wide transcriptional dynamics.

These data provide a foundation not only to support the utilization of *C. beijerinckii* in industrial ABE fermentation from lignocellulosic substrates but also to understand its physiological changes in the presence of inhibitory compounds.

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IN-DEPTH INSIGHTS INTO ESTABLISHING PROGRAMMABLE AND EFFICIENT AUTOLYSIS FOR *PSEUDOMONAS PUTIDA* BIOTECHNOLOGY

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Efficient release of intracellular cargo remains a major bottleneck in biotechnological applications of Gram-negative bacteria due to their double-membrane envelope. This limitation restricts production systems based on intracellular product accumulation and is particularly relevant in *Pseudomonas putida*, a versatile laboratory and industrial host. Although programmable autolytic systems offer a strategy to overcome secretion barriers, their performance has mainly been studied in *Escherichia coli*, with limited understanding of their dynamics, efficiency and context dependence in alternative cell factories.
To address this gap, we systematically compared three engineered lytic modules in *P. putida* – EstPbeta (an outer membrane-disrupting autotransporter), Enlys (a prophage-derived endolysin) and ColE3 (a colicin targeting 16S rRNA). These systems were evaluated in wild-type KT2440 strain and its genome-reduced derivatives EM371 and EM42 to assess the impact of genomic background on autolysis dynamics.
The lytic efficiency was strongly influenced by induction timing, host genomic context, and mechanism of action. Reduced lysis upon late-log induction appears to be associated with insufficient expression rather than intrinsic enzymatic limitations. Since maximal intracellular cargo accumulation is typically reached upon entry into stationary phase, reprogramming using stationary-phase promoters is currently being evaluated as a strategy to enhance autolytic performance while preserving biomass build-up.
Taken together, this work offers valuable insights into the host-circuit interactions that govern programmable autolysis in *P. putida* strains and highlights key biological constraints that must be considered when developing strategies for controlled cell disruption. We also recognize the limitations of conventional synchronous single-event lysis and are therefore currently exploring asynchronous lysis concepts as a potential approach to enable sustained cargo release without complete culture collapse.

PHANTASTIC ENZYMES AND WHERE TO FIND THEM

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PolyHydroxyAlkanoate (PHA) synthases represent key enzymes in the synthesis of versatile biopolymers with potential to change plastics industry. Although PHAs are relatively widely studied, much less is known on particular genes coding those key enzymes responsible for their synthesis. Their analysis is hampered by their diverse primary structure as it is difficult to infer orthologous relationships correctly. During the last several years, we sequenced, assembled, and analyzed various genomes of PHA-producing bacteria, e.g., *Caldimonas thermodepolymerans*, *Caldimonas aquatica*, *Tepidimonas taiwanensis*, *Aneurinibacillus thermoaerophilus*, and others. In addition, we used our experience from the analysis of these thermophilic bacteria to screen already available genomes of other thermophilic bacteria as well as archaea. Finally, we moved our attention to other groups of bacteria and we are currently sequencing additional 50 genomes of organisms producing PHA, including psychrophilic ones. Their initial screening will help us to design adjusted computational pipelines to screen thousands of additional available genomes in order to identify novel PHA synthases.

This study was funded by the Czech Science Foundation (GACR) (Project No. GM25-17459M).

CHARACTERIZATION OF PHA SYNTHASE AND PHA DEPOLYMERASE ENZYMES FROM THE THERMOPHILIC BACTERIUM *CALDIMONAS THERMODEPOLYMERANS*

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Polyhydroxyalkanoates (PHAs) are microbial polyesters that represent a sustainable alternative to fossil fuel-based plastics. These biodegradable polymers have properties similar to conventional plastics and can be produced from waste materials. PHA synthase is a key enzyme in PHA synthesis, while PHA depolymerase is essential for biodegradation. Despite their importance, only a few have been characterized in detail.

We characterize these enzymes from the thermophilic bacterium *Caldimonas thermodepolymerans*, an attractive candidate for PHA production due to its unique properties such as utilization of xylose-rich substrates and high PHA yields

(up to 87% CDW). Using bioinformatic tools, we predicted the secondary and tertiary structures of both enzymes including their active sites. PHA synthase was successfully expressed in *E. coli*, purified and its enzymatic activity was confirmed. The predicted active site residues of PHA synthase were validated by site-directed mutagenesis and an activity assay. Further characterization included determination of the enzyme's pH and temperature optima as well as its thermal stability. Additional biophysical characterization is ongoing. The characterization of PHA depolymerase is challenging, as in *E. coli* it is produced in an insoluble form and efforts to improve its solubility have been unsuccessful so far. Our work represents one of the first efforts to dissect molecular properties of PHA (de)polymerizing machinery of thermophilic bacterium.

BIOTECHNOLOGICAL POTENTIAL OF IRON-ENRICHED YEAST BIOMASS FOR THE PRODUCTION OF BIOACTIVE METABOLITES

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Yeasts represent a diverse group of microorganisms capable of producing a broad spectrum of nutritionally and biologically valuable metabolites, including antioxidants and compounds with antimicrobial activity. One major advantage of cultivating these microscopic fungi lies in their metabolic flexibility and ability to utilize a wide range of nutrient sources. This feature enables the integration of yeast cultivation into circular economy strategies, for example through the use of waste-derived substrates, while simultaneously influencing the production of valuable metabolites.
The present study focuses on the enrichment of yeast biomass with biogenic elements, with particular emphasis on iron. In addition to influencing the biosynthesis of important metabolites, microbial biomass can accumulate micro- and trace elements in activated or directly bioactive forms. In the case of iron, these forms include various chelates, bisglycinates, and structures resembling heme complexes. This ability makes enriched yeast biomass a promising source for the production of dietary supplements or pharmaceutical preparations aimed at individuals suffering from disorders associated with iron deficiency, such as anemia, where iron supplementation plays an important therapeutic role.
Furthermore, the increased availability of selected elements may influence the biosynthesis of metabolites with antimicrobial properties, which naturally serve as protective compounds for microorganisms in competitive environments.
Metabolites present in the yeast biomass were analyzed using several analytical techniques, including gas chromatography (GC) and high-performance liquid chromatography (HPLC). The accumulation of supplemented micro- and trace elements in the biomass was determined using inductively coupled plasma optical emission spectrometry (ICP-OES).

The results of this study may provide valuable insights for the application of enriched yeast biomass in industrial biotechnology and support the development of economically efficient and sustainable production strategies.

ENDOPHYTIC *BACILLUS ATROPHAEUS* AS A PROMISING SUSTAINABLE BIOCONTROL AGENT AGAINST FUNGAL PHYTOPATHOGENS

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Fungal phytopathogens cause substantial global crop losses and represent a major obstacle to sustainable food production. Growing concerns regarding the environmental and health risks associated with synthetic fungicides have intensified interest in biological control strategies. This motivates the screening of endophytic bacteria, integral members of plant microbiomes, for both plant-growth-promoting (PGP) traits and antifungal activity. An endophytic strain identified by 16S rRNA gene sequencing as *Bacillus atrophaeus* was isolated from *Populus alba* L. and qualitatively compared with endophytes from *Triticum aestivum* L. and *Ficus carica* L. using *in vitro* PGP trait assays**.** *B. atrophaeus* exhibited strong amylase and protease activity and ammonia production, robust biofilm formation, and evidence of nitrogen fixation. Notably, it was the only strain exhibiting chitinase activity, a key antifungal trait. In dual-culture assays on Potato Dextrose Agar, *B. atrophaeus* strongly inhibited a broad range of phytopathogenic fungi, with inhibitory levels at more than 60%, and outperformed the other tested bacteria. Cell-free supernatant containing extracellular antifungal metabolites also significantly reduced fungal growth, with near-complete inhibition of *Sclerotinia sclerotiorum* at early time points. However, inhibition decreased with prolonged incubation, suggesting partial instability of these metabolites. Antifungal activity varied with bacterial growth phase and carbon source, with the complex, nutrient-rich Luria–Bertani medium yielding approximately twofold greater inhibition than a minimal medium supplemented with xylose as the sole carbon source. Overall, these results position *B. atrophaeus* as a promising candidate for development as a sustainable biocontrol agent.

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IMPACT OF FUMARIC ACID-CHITOSAN APPLICATION ON AROMA COMPUNDS IN TOKAJ WINES AS A SUSTAINABLE BIOPROTECTION STRATEGY FOR REDUCING SULFUR DIOXIDE USE

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Bioprotective technologies using microbial metabolites represent an emerging biotechnological direction for reducing sulphur dioxide in winemaking, supporting current efforts to replace or minimise SO_2 through scientifically grounded alternatives [1]. In this study, the biotechnological potential of a fumaric acid–chitosan formulation (EnartisStab Micro Zero) was evaluated in botrytised Furmint musts from the Tokaj region. Chitosan derived from *A. niger*, combined with fumaric acid, offers a dual-action metabolite-based strategy that enhances chemical robustness, stabilises must composition and contributes to more predictable fermentation outcomes, consistent with modern bioprotection frameworks [2,3]. Musts were treated with different dosages of the preparation, with and without reduced SO_2. GC–MS HS-SPME analysis identified 87 volatile compounds, showing that the fumaric acid–chitosan treatment selectively modulated key aroma pathways: fruity esters such as ethyl octanoate decreased, while floral and honey-like markers including 2-phenylethanol, phenylethyl acetate and damascenone increased, enhancing the varietal and botrytised character of Furmint. Sensory profiling confirmed improvements in aroma purity, roundness and overall harmony, particularly at 40 g/hl combined with minimal SO_2. These results underline the biotechnological relevance of fumaric acid–chitosan application as a sustainable tool that reduces sulphur dioxide requirements while positively influencing aroma development, supporting the transition toward metabolite-driven, low-input winemaking technologies.

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OPTIMIZED PARAMETRIC STUDY OF WATERMELON SEED OIL BIODIESEL PRODUCTION VIA KAOLIN-SUPPORTED ZEOLITE CATALYSIS

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Abstract
In line with the Fourth Industrial Revolution (4IR) drive, Nigeria just like the rest of the world is desirous of moving towards a circular and resource-efficient economy, with renewable energy at the centre of this transition. Watermelon seeds, often discarded as agricultural waste, are a readily available by-product that can be valorized through biodiesel production. Producing biodiesel from watermelon (Citrullus lanatus) seed oil in Nigeria has the potential to reduce dependence on imported petroleum products, offers a locally sourced energy alternative, boost energy security, helps stabilize fuel availability, reducing greenhouse gas (CO_2) and pollutant emissions. In converting watermelon seed oil to biodiesel, zeolites enhance the transesterification process by improving reactant diffusion, increasing conversion efficiency, and producing higher-purity fuel. This work aims to study the effects of key process variables in producing biodiesel from watermelon seed oil using a kaolin-based zeolite as a catalyst. The transesterification was optimized by varying the reaction time, methanol-to-fatty acid molar ratio, reaction temperature, and catalyst concentration using the Response Surface Methodology (RSM). It was discovered that the highest yields (92 % and 93 %) for predicted and actual values, respectively were obtained at the following conditions: methanol to oil ratio of 4.5:1, catalyst loading of 0.75 g, reaction temperature of 65 ^{o}C, and reaction time of 105 mins, with R^2 values of 0.9510. Comparison of the obtained biodiesel quality with relevant ASTM standards showed promising results, with kinematic viscosity, cetane number, flash point, and free fatty acid of 4.4 mm^2/s, 62.4, 156 °C, and 0.37, respectively within acceptable range of values.

HOW CAN FIRST GENERATION BIODIESEL REFINERY SURVIVE YEAR 2030?

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Though there is an immense political support to utilise waste based raw material for advanced biofuels, there is not enough raw material available. Then oilseeds, particularly rape and canola seeds, are still most important source of raw material to fulfil Green Deal objectives in transport. To be able to survive beyond 2030 deep restructuring is inevitable for first generation biodiesel plant as presented below.

It is a must for any fuel refinery to succeed in maximised yield of fuel, minimised utility consumption and close to zero waste generation. Next to that biofuel refinery of the future will have to consume raw materials and utilities with very low GHG footprint and efficiently reprocess organic waste and side-streams. Comparing to advanced biofuel plants, based on e.g. cooking oil supplies, first generation biofuel operator has an advantage of having available organic waste and low value side-streams that have potential to be further processed. In fact, it is huge opportunity to install technology that is further processing waste and side-streams to produce green energy and generate product with highly negative GHG emissions. If such a product is sellable on the market it provides not negligible contribution to the overall refinery economics.
Moreover management of biofuel refinery has to go outside of their fence and look at the options how to decrease emissions from oilseed plantation via e.g. cooperation with fertiliser producer. As nitrogen release to the open air and underground water is main contributor to the emission level from plantation a way of fixing of such a release is important. Usage of advanced fertiliser based on biodiesel plant newly produced side-product as a barrier enables slow release of nitrogen in the course of plant growth and thus leads to decrease of GHG emissions from plantation even lower then to one half. Taking into account overall balance of GHG emissions then such a biodiesel fuel has a potential to meet net zero target.
An example of rape - seed based biodiesel refinery with optimised processes, fully green utilities and valuable side-product that sinks huge portion of carbon to achieve such a goal is presented.

BIOECONOMY AS A STRUCTURAL CARBON MANAGEMENT INSTRUMENT IN TRANSPORT AND THE CHEMICAL INDUSTRY

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The decarbonisation of the European economy is often primarily associated with electrification. However, in a number of transport and industrial segments, full electrification is neither technologically nor economically feasible. In areas requiring high energy density or molecular carbon – such as heavy-duty transport, aviation, and the chemical industry – renewable carbon remains structurally indispensable.
This contribution presents the bioeconomy as a long-term carbon management strategy rather than a transitional solution. Based on an analysis of the bio-based sector, it demonstrates how renewable carbon flows can be integrated into fuel and chemical value chains while simultaneously complying with the requirements of RED III and related methodologies for calculating greenhouse gas emission savings.

The paper focuses on the technological readiness of advanced pathways, the role of digital emissions reporting (LCA, GHG), and the impact of regulatory stability on investment decision-making. The case of a small open EU economy illustrates how methodological changes and regulatory uncertainty influence the pace of capacity development.
The bioeconomy can therefore represent a structural pillar of the European decarbonisation strategy, provided it is supported by methodological consistency and a predictable regulatory framework.

INDUSTRIAL IMPORTANCE AND SYNTHESIS OF E-CAPROLACTONE

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The growing demand for sustainable materials has significantly increased the importance of ε-caprolactone in both research and industrial contexts. ε-Caprolactone is a seven-membered cyclic ester that serves as a key platform molecule in modern polymer chemistry. Its primary industrial relevance arises from its use as a monomer for the production of poly(ε-caprolactone) (PCL), a biodegradable and biocompatible polyester with versatile application potential. PCL is widely used in biomedical engineering, e.g., tissue scaffolds, drug delivery systems, and resorbable medical devices, as well as in packaging and advanced composite materials. Its flexibility, processability, and controlled biodegradability make PCL one of the most promising aliphatic polyesters for high-value applications.
The development of efficient and sustainable ε-caprolactone synthesis routes represents an important technological objective. Advancements in ε-caprolactone production technologies directly impact the economic viability of biodegradable polymer manufacturing and contribute to the broader transition of the chemical industry toward greener and more energy-efficient processes. In this work, a batch bioreactor for biopolymer production was designed. Calculations are based on kinetic parameters from literature. These data were used to simulate the course of a four-step cascade reaction. Obtained results enabled the determination of key bioreactor parameters and an estimation of the process economics.

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BIOTECHNOLOGY AND BIOREFINERY

POSTERS

COMPLETE UTILISATION OF BREWERY BY-PRODUCTS FOR THE FORMULATION OF A FUNCTIONAL DIETARY SUPPLEMENT

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The brewing industry generates substantial amounts of by-products, primarily brewer's spent grain, spent hops, and residual yeast biomass. These materials are traditionally used as low-value animal feed or discarded, despite their significant nutritional and bioactive potential. The aim of this study is to introduce the utilisation of these brewery by-products in the production of a functional dietary supplement intended for human consumption.
Brewer's spent grain represents a rich source of dietary fibre, particularly insoluble components, which contribute to improved gastrointestinal health and metabolic regulation. Spent hops are rich in phenolic compounds and other bioactive substances with high antioxidant activity. Finally, brewer's yeast biomass provides valuable nutrients, including proteins, B-complex vitamins, and biologically active β-glucans known for their immunomodulatory properties.
The proposed concept integrates these three by-products into a functional dietary supplement formulation that combines fibre, antioxidants, and micronutrients.
This contribution presents possible approaches to the treatment of particular components, including hydrolysis, fermentation, autolysis, and extraction, followed by their compilation and final processing into powder and tablets for nutritional and functional preparation.
The presented concept shows how brewery waste streams can be converted into valuable products with potential health benefits, while also supporting circular economy principles in the brewing sector.

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OPTIMISATION OF HYDROLYTIC PROCESSING OF BREWER'S SPENT GRAIN FOR BIOTECHNOLOGICAL APPLICATIONS

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With increasing pressure on the principles of the circular economy and sustainable resource use, there is also growing interest in the biotechnological utilisation of by-products from the agricultural and food industry. Brewer's spent grain (BSG) is a significant by-product of the food industry that has the potential to be further biotechnologically

valorised into more valuable, functional and nutritious products. This is primarily due to the fact that BSG is an inexpensive yet valuable source of carbon, nitrogen and other minerals that can be utilised by microorganisms.

BSG is composed of lignocellulose, hemicellulose, and lignin. These compounds give BSG a highly compact and complicated structure that is potentially hard for microorganisms to access and utilise. Nevertheless, by selecting the suitable hydrolytic or enzymatic conditions, we are able to disrupt this complex structure and release monosaccharides, such as glucose, xylose and arabinose, which can then be utilised by microorganisms. However, disruption can also lead to the formation of lignocellulose-derived inhibitors, which can hinder microbial growth.

Having successfully optimised the conditions for enzymatic hydrolysis, we are now focusing on further optimising the acid pretreatment from an environmental perspective. Specifically, our aim is to carry out the hydrolysis step solely under acidic conditions, thus eliminating the need for enzymatic treatment. This approach could simplify the entire process and reduce costs. In addition, the potential of the combination of pretreated hydrolysate and waste brewer's yeast as a nutrient source was investigated. To determine the nutritional value of waste brewer's yeast, its total polyphenol content was evaluated and compared with commercially available yeast, as brewer's yeast contains various beer-derived compounds, including polyphenols that may interfere with microbial growth.
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SYNTHESIS OF BIO-EPOXIDES BY ENZYMATIC AND HOMOGENEOUS CATALYSIS

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Epoxidized fatty acid methyl esters (FAME) are versatile bio-based intermediates for polymers, coatings and lubricants. This work compares lipase-mediated chemoenzymatic epoxidation with conventional homogeneous peracid epoxidation using rapeseed-oil FAME as substrate. Several microbial lipases, applied in soluble form and after covalent immobilization on various solid supports, were screened under identical reaction conditions (40 °C, H_2O_2 concentration). Although all preparations were hydrolytically active, only the commercial Novozyme 435 (immobilized *Candida antarctica* lipase B) produced, under the selected reaction conditions, detectable epoxides. Epoxide formation was confirmed by the appearance of oxirane bands in FTIR spectra and by GC/MS, which showed a time-dependent decrease of unsaturated esters and the emergence of mono- and diepoxidized derivatives. The influence of reaction time (4–24 h) and oxidant-to-double-bond molar ratio (0.75–2.00) demonstrated that controlled peroxide dosing is required to increase conversion while preserving selectivity; excessive oxidant altered

product composition. Benchmarking against a formic acid/H_2O_2 homogeneous system (60 °C, 3 h) revealed faster conversion but a broader product distribution, consistent with enhanced side reactions. In contrast, Novozyme 435 enabled gradual epoxidation under mild conditions and offered improved control over product composition. These findings underline the critical role of enzyme formulation and immobilization in oxidative chemoenzymatic processes and support enzymatic epoxidation as a selective, more sustainable route to bio-epoxides.

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THE TRICK IS MAKING IT COME BACK: POLYMER DEGRADABILITY IN SOIL AND MICROBIAL PRODUCTION OF PHB

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Abstract
Biodegradable polymer mulching foils are considered a potential way to reduce the accumulation of persistent plastic residues in agricultural soils; however, their actual degradation behavior and interactions with soil microorganisms still require careful assessment. This study aims to explore the soil degradation of biodegradable polymer fragments (as a model of mulching-foil residues), focusing on polyhydroxybutyrate (PHB), and polylactic acid (PLA) and using the degradradation product (such as lactic acid, 3-hydroxybutyrate) to produce new PHA via microbial consortium in soil. The aim is to make a circle of the synthesis, applications and polymer end-of-life – to make real that one man's trash could be bacteria's treasure.
Fragments of mulching foils were incubated in agricultural soil to approximate field exposure conditions. After incubation, residual polymer fragments were recovered via density separation and analyzed as resting materials using physico-chemical methods to examine potential changes in their properties. Soil-derived bacterial communities were cultivated to assess their ability to produce intracellular polyhydroxyalkanoates (PHA), and polymer biosynthesis was verified using FTIR and gas chromatography, which enabled the detection of PHA.
The results indicate that soil microorganisms may not only contribute to the degradation of biodegradable mulching foils but could also, under suitable conditions, synthesize biopolyesters from available carbon sources. These observations suggest that soil functions as an active biological environment influencing polymer transformation, and

they point toward the potential – though not yet fully verified – role of biodegradable mulching materials.
This study was financed by GAČR project GA25-18143S.

DEVELOPMENT OF AN ANTIFUNGAL AGENT EFFECTIVE AGAINST THE PATHOGENIC FUNGUS *VERTICILLIUM*

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Every year, agriculture faces a decline in crop-planted areas, but also lower yields caused by many types of pathogens that usually kill plants. Among them, *Verticillium* fungus is one of the most aggressive pathogens responsible for verticillium wilt, which attacks plant roots and causes them to wilt by blocking water transport through the infected plant, leading to its death. This poses a huge problem for agriculture, as there are few or no agents that can cure plants and eradicate the fungus. The hope for treating plants lies in a biological agent effective against fungi based on viable bacteria that produce many secondary metabolites with antifungal activity. The bacterial agent could be grown in waste hydrolysates, such as feather hydrolysates, to reduce the cost of future production of the agent with minimal environmental impact. There are several bacterial candidates that have shown potential to become possible bioactive agents for protecting plants against phytopathogens such as *Verticillium* in the future, and some of them also promote plant growth.

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PHA SYNTHASE AND ITS MANY RELATIVES

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Polyhydroxyalkanoates (PHAs) are biodegradable, biocompatible, and renewable polyesters produced by microorganisms as intracellular carbon and energy storage compounds. Owing to these properties, PHAs are considered promising alternatives to fossil-based plastics. While genome sequencing has become routine, the functional annotation of biosynthetic pathways remains a bottleneck in revealing microbial metabolic potential. This is especially true for PHA synthases, the enzymes responsible for PHA biosynthesis. Many potential PHA synthases remain unrecognized because they are

frequently annotated as hypothetical proteins rather than *phaC* homologs. To address this issue, we screened all bacterial and archaeal reference genomes available in RefSeq using DELTA-BLAST with representatives of all currently known PHA synthase classes as query sequences. The analysis uncovers multiple candidate homologs that may represent previously unrecognized PHA synthases and suggests that the diversity of these enzymes in prokaryotes is currently underestimated.

This study was funded by the Czech Science Foundation (GACR) (Project No. GM25-17459M).

EFFECT OF FOOD INDUSTRY BY-PRODUCTS ON THE GROWTH DYNAMICS OF SELECTED YEAST GENERA

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The study investigates the potential use of food industry by-products, specifically whey and spent coffee grounds, as substrates for yeast cultivation. These materials represent abundant waste streams that can be valorised within the framework of a circular economy. Prior to their use, both substrates require appropriate pretreatment to improve their suitability for microbial metabolism. Whey is a complex substrate of animal origin that provides both carbon and nitrogen sources. In contrast, spent coffee grounds represent a plant-derived material that must be pretreated by acidic followed by enzymatic hydrolysis, enabling the release of fermentable carbohydrates while retaining sufficient nitrogen content for cultivation purposes.
Yeasts are widely used in biotechnology due to their metabolic versatility and their capacity to perform biotransformation of various substrates into valuable metabolites. Their metabolic activity can be utilized to convert waste biomass into valuable products such as lipids, vitamins, polysaccharides, or microbial biomass. In this study, two yeast strains representing different taxonomic groups were used: the ascomycetous yeast *Metchnikowia pulcherrima* and the basidiomycetous yeast *Cystofilobasidium infirmominiatum*.
The objective of this work was to evaluate the influence of waste-derived substrates on yeast biomass formation and growth dynamics. Different ratios of the tested substrates were applied to examine their effect on key growth parameters, including the duration of the lag phase and the intensity of growth during the exponential phase. Understanding these responses may support the development of sustainable biotechnological processes utilizing waste substrates for yeast cultivation.

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ANTIBACTERIAL EFFECTS OF FOOD-GRADED *MONASCUS* PIGMENTS ON *CLOSTRIDIUM BUTYRICUM*

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Monascus species are traditional edible and medicinal fungi with a history of more than 2,000 years of use. During fermentation on rice or other substrates, they produce a wide range of secondary metabolites (SMs), including Monascus pigments (MPs) used as natural food colorants. Compared with synthetic colorants, natural pigments derived from Monascus spp. are more environmentally friendly and readily obtainable, leading to their widespread application in the food industry. Food-grade Monascus pigments have been reported to exhibit both vivid coloration and antibacterial activity, particularly against Gram-positive bacteria. In this study, the growth of Clostridium butyricum NBRC 13949 was evaluated following the addition of crude MP extracts with different compositions derived from various strains and culture media. The results demonstrated that MPs inhibited the growth of C. butyricum, with stronger inhibitory effects observed when cultures were inoculated with fresh vegetative cells. Compared with the control group, MP treatment imposed growth stress on C. butyricum, resulting in prolonged cell morphology. UHPLC analysis of the crude MP extracts indicated that the yellow pigment fraction was primarily responsible for the observed antibacterial activity against C. butyricum.

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FUNCTIONALIZED CROSSLINKED HYALURONIC ACID NANOPARTICLES FOR CELLULAR IMAGING AND RADIOPROTECTION

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Hyaluronic acid (HA) is a naturally occurring biopolymer widely distributed in the human body, particularly in the extracellular matrix of connective tissues, skin, joints, and cartilage. Owing to its excellent biocompatibility, HA has been extensively investigated for various biomedical applications. However, the use of soluble HA is limited by its rapid

degradation and fragmentation into low-molecular-weight pro-inflammatory fragments, mediated by reactive oxygen species (ROS) and hyaluronidases.
To address these limitations, we prepared crosslinked HA nanoparticles (HANPs) exhibiting enhanced structural stability and resistance to degradation [1-2]. The presence of reactive functional groups (carboxyl and hydroxyl groups) along the HA backbone enables further chemical modifications of HANPs with bioactive molecules.
In this study, HANPs were functionalized with a fluorescent label and with amifostine, including its active metabolite WR-1065. Fluorescent labeling enabled the investigation of cellular interactions, specifically to evaluate receptor-mediated binding to CD44 and potential cellular internalization. Amifostine is a clinically used radioprotective agent that reduces the toxicity of radiotherapy and chemotherapy in patients with various malignancies, including lung, ovarian or breast cancer. Its protective effects involve mitigation of damage to healthy tissues such as the kidney, bone marrow, heart and other healthy tissues [3]. As HA has also been reported to exhibit radioprotective properties, its combination with amifostine may provide a synergistic strategy to enhance tissue protection during cancer treatment [4].

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VALORIZATION OF LIGNOCELLULOSIC WASTE FOR PHA PRODUCTION USING THE THERMOPHILE *CALDIMONAS THERMODEPOLYMERANS*

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In recent years, there have been major advances in industry which, in addition to improving the quality of everyday life, has also caused massive enviromental pollution such as plastic pollution. This issue could be solved by replacing the petrochemical plastics in certain fields by in nature biodegrable materials such as polyhydroxyalkanoates (PHAs). PHAs can be produced by various microbial producers for example by thermophilic bacterium *Caldimonas thermodepolymerans*. This thermophile is very promising due to is ability to grow on xylose as a carbon source. This ability to utilize xylose opens up the possibility of using lignocellulosic waste from the agricultural industry as a carbon source

to reduce the cost of PHA production. This study examines the process of preparing hydrolysate from wheat residues (straw) using acid and thermal hydrolysis employing oxalic acid. Hydrolysates were prepared using this method because the use of oxalic acid breaks down hemicellulose, resulting in a hydrolysate with a high proportion of xylose and a minimum amount of glucose, which *Caldimonas thermodepolymerans* is unable to metabolize. After optimizing the hydrolysis preparation conditions (e.g., time, temperature, etc.) and subsequent analysis using HPLC different methods of detoxification of hydrolysates by extraction with suitable solvents were also tested. After that, the hydrolysate containing the highest concentration of xylose was used as a carbon source for the production of PHAs by *Caldimonas thermodepolymerans* bacterium.

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HYDROLYSATES FROM WASTE BIOMASS AS A HIGH-QUALITY ORGANIC FERTILIZER

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Hydrolysates derived from otherwise unusable animal production waste represent a sustainable (environmentally friendly, cost-effective) alternative for utilizing difficult-to-process materials with added value potential. In agriculture, for example, they can serve as valuable inputs for the formulation of fertilizers, bio-stimulants, or plant stress-protection products.
The effect of a mixed hydrolysate applied as a foliar treatment was tested on field crops, specifically winter wheat, at selected plant growth stages. A particularly positive effect was observed on the number and weight of grains per ear when applied once or twice during vegetation at a dose of 4–8 L/ha. This can result in an increase in crop (cereal) yields of up to 2–8%.

Keywords: animal waste hydrolysates, bio-stimulation, foliar application, cereals.

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CLICK ME IF YOU CAN: WILD-TYPE *ANEURINIBACILLUS* AS SURPRISING ARCHITECTS OF FUNCTIONAL PHA COPOLYMERS

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Polyhydroxyalkanoates (PHAs) are promising biodegradable alternatives to conventional plastics, yet their material properties are often limited by the narrow range of monomers incorporated by natural microbial producers. Here, we demonstrate the remarkable ability of wild-type *Aneurinibacillus* spp., isolated from compost and activated sludge, to biosynthesize structurally diverse and functional PHA copolymers without any genetic modification.

When cultivated on glucose (4 g/L) supplemented with structurally distinct co-substrates, particularly lactones and diols (4 g/L), these thermophilic strains incorporated a broad spectrum of PHA monomers, including 3-hydroxyvalerate, 4-hydroxyvalerate, 5-hydroxyvalerate, 4-hydroxybutyrate, and 4-hydroxyhexanoate, highlighting the remarkable substrate tolerance of their native PHA synthases. Cultivation with α-methyl-γ-butyrolactone led to the formation of the terpolymer poly(3-hydroxybutyrate-co-3-hydroxyvalerate-co-4-hydroxy-2-methylbutyrate), containing the very rare α-methyl-branched monomer 4-hydroxy-2-methylbutyrate, a structural motif only exceptionally reported in natural PHAs.

Material characterization of the obtained copolymers revealed reduced crystallinity and increased flexibility compared to poly(3-hydroxybutyrate), indicating a more amorphous polymer structure with desirable material properties and improved processing potential.

Exploiting the inherent alcoholytic activity of class IV PHA synthases, terminal alkyne-functionalized alcohols and polyethylene glycol (PEG) were supplied during cultivation to modify PHA chain ends. Alkyne-functionalized alcohols introduced terminal triple bonds suitable for further post-synthetic functionalization via click chemistry, whereas PEG acted as a hydrophilic modifier, generating amphiphilic PHA materials. Their incorporation and polymer structure were primarily confirmed by NMR spectroscopy, while SEC-MALS revealed decreased molecular weight consistent with alcoholysis-mediated chain scission and end-group capping.

USING MICROBIAL EXTRACTS TO CREATE COSMETICS PRODUCTS

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This study aimed at the development of cosmetic formulations incorporating microbial extracts while simultaneously exploring the valorisation of food industry by-products, specifically spent coffee grounds, as an alternative cultivation substrate. The primary objective was to convert this waste material into value-added bioactive metabolites with potential cosmetic applications and to characterize these compounds analytically.
The investigated metabolites comprised fatty acids, carotenoids, polyphenols, and flavonoids. The antioxidant and antimicrobial properties of the prepared extracts were assessed using the model bacterial strains *Escherichia coli* and *Staphylococcus epidermidis*. Based on the obtained results, an appropriate cosmetic formulation containing the microbial extracts was selected.
The experimental work included yeast cultivation and co-cultivation with microalgae to enhance the spectrum of bioactive compounds. The microbial strains employed were *Phaffia rhodozyma* CCY 77-1-1, *Cystofilobasidium macerans* CCY 10-1-2, *Rhodosporidium toruloides* CCY 062-002-004, and *Chlorella vulgaris* CCALA 924. Extracts were prepared from both monocultures and the co-culture of *Phaffia rhodozyma* and *Chlorella vulgaris*, with biomass combined in equal proportions (1:1) for the final extract preparation.
The resulting cosmetic product was formulated as a body scrub enriched with microbial extracts and residual spent coffee grounds. Coffee oil derived from the waste material was utilized during microbial cultivation, while the remaining solid fraction was incorporated into the scrub formulation, enabling comprehensive waste utilization within the production process.

Acknowledgments
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THE PATH TO SUSTAINABLE NUTRITION: ISOLATING ALTERNATIVE PROTEINS FROM RESIDUAL BIOMASS

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In recent years, modern lifestyles have led to growing global demand for sustainable and environmentally friendly sources of protein to supplement or replace animal sources. Yeast and microalgae are ideal candidates for this purpose. However, in current

biotechnological practice, they are often cultivated primarily for the production of specific exogenous substances, such as exopolysaccharides, while the remaining biomass is often considered unused waste.

First stepi is to subjest the biomass to lipid extraction using organic solvents or more sustainably via Supercritical Fluid Extraction (SFE) using CO_2. The core of this work is the optimization of the protein extraction process from the residual biomass. The study focuses on the optimization of alkaline extraction, where key factors such as pH, temperature, and extraction time were experimentally investigated to maximize yield while maintaining high isolate quality. In addition, for selected algae and cyanobacteria, a gentle phycocyanin extraction step was integrated into the process prior to the alkaline phase itself, preventing its degradation and capturing an additional high-value bioactive pigment.Once the proteins and lipids have been isolated, the remaining solid fraction consists primarily of structural carbohydrates (such as glucans or cellulose). This carbohydrate-rich residue can be than used for other applications.

The result of this experiments could be a practical, optimized protocol that enables the efficient valorization of microbial production residues through a cascade of separation steps. It supports the principles of the circular economy in biotechnology. By utilizing every component of the cell—from lipids and pigments to proteins and sugars—we contribute to a truly sustainable production model for future generations.

This study was carried out with the support of the long-term conceptual development of a research organization the Faculty of Chemistry, Brno University of Technology, Project No.FCH-S-26-9000.

PUSHING THE 3HV BOUNDARY: ENGINEERING *CALDIMONAS THERMODEPOLYMERANS* FOR PHAS COPOLYMERS

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Polyhydroxyalkanoates (PHAs) are natural polyesters synthesized by numerous bacteria as intracellular energy storage compounds and represent promising biodegradable alternatives to petroleum-based plastics. The material properties of PHA-based bioplastics strongly depend on their monomer composition; therefore, copolymers are often preferred due to their closer resemblance to conventional petrochemical plastics. To tailor polymer composition, genetic modification strategies are employed to redirect metabolic fluxes toward enhanced PHA biosynthesis and controlled incorporation of specific monomers into the poly(3-hydroxybutyrate) (P3HB) backbone.

In this study, we present a deletion mutant derived from *Caldimonas thermodepolymerans* DSM 15344 constructed via homologous recombination. The engineered strain, *C. thermodepolymerans* KS01, sequentially carries deletions of three restriction endonuclease genes, the gene encoding PHA depolymerase, and the gene encoding 2-methylcitrate synthase. The removal of restriction endonuclease genes was performed to improve genetic accessibility and facilitate further genome engineering. Subsequent deletion of the PHA depolymerase gene was aimed at preventing intracellular polymer degradation and thereby increasing the molecular weight of the accumulated PHA. Finally, deletion of the 2-methylcitrate synthase gene was designed to redirect propionyl-CoA metabolism toward enhanced 3-hydroxyvalerate (3HV) biosynthesis. As a result of these combined modifications, the mutant strain exhibits improved PHA accumulation together with elevated incorporation of 3HV into the copolymer. Importantly, these metabolic features are complemented by the intrinsic physiological advantages of *C. thermodepolymerans*, a thermophilic bacterium capable of high-cell-density cultivation and efficient xylose utilization. These characteristics make the strain particularly attractive for the valorization of lignocellulosic hydrolysates and for sustainable, large-scale bioprocess applications.
To evaluate the strain's capacity for 3HV incorporation, selected precursor substrates (sodium propionate, valeric acid, and levulinic acid) were supplemented at different concentrations and time points during the production phase. The effects of precursor feeding strategies on cell growth, PHA accumulation, and monomer composition were systematically monitored to determine optimal conditions for enhanced 3HV incorporation. These findings contribute to the development of tailored PHA copolymers with improved material properties suitable for sustainable bioplastic applications.

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PRODUCTION AND BIOLOGICAL EVALUATION OF YEAST-DERIVED EXTRACELLULAR POLYMERIC SUBSTANCES

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Extracellular polymeric substances (EPS) produced by yeasts represent a structurally diverse group of biopolymers with increasing potential in food, pharmaceutical, and biotechnological applications. These extracellular polymers contribute to microbial protection against environmental stress and participate in the formation of extracellular matrices. Compared with bacterial polysaccharides, yeast-derived EPS offer advantages such as relatively high production yields, simpler downstream processing, and diverse biological activities. However, their production efficiency, chemical composition, and functional properties remain insufficiently explored.

The aim of this study was to evaluate EPS production by yeast cultures and to characterize their biochemical composition and biological properties. Yeasts were cultivated under controlled conditions, and EPS were isolated from the culture medium using precipitation-based methods. Biomass formation and EPS production were determined gravimetrically, while the chemical composition of the polymers was analyzed with respect to their main structural components.

The biological activity of the isolated EPS was further evaluated through cytotoxicity assays using human intestinal epithelial cell models and by assessing their prebiotic potential based on the growth stimulation of selected probiotic microorganisms.

The results indicate that yeast cultivation enables the production of structurally complex EPS alongside significant biomass formation. The isolated polymers showed no cytotoxic effects on intestinal cell models and supported the growth of probiotic bacteria, suggesting potential prebiotic activity.

Overall, the study highlights yeast-derived EPS as safe and biologically active biopolymers with promising potential for applications in functional foods and biotechnology.

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POLYMERS AND COMPOSITES

LECTURES

INVESTIGATION OF NATURAL RUBBER PROCESSING: TESTING, EVALUATION, AND COMPARATIVE ANALYSIS

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The relationship between laboratory methods for evaluating rubber processability and actual processing operations was investigated using natural rubber samples from a single African plantation. Conventional tests defined by the Standard Malaysian Rubber (SMR) specification, including Wallace plasticity and Mooney viscosity, are commonly used to assess processability; however, these methods operate at relatively low shear rates ($\approx 1\ s^{-1}$). In this study, the standard measurements were extended by a modified Mooney viscosity test performed at a shear rate below $0.2\ s^{-1}$ to enhance sensitivity to the microstructure of natural rubber and reduce melt fracture effects. Additional rheological measurements were conducted using a rheological extrusion die operating at high shear rates typical of industrial processing. Viscoelastic properties were further characterized using an RPA rheovulcameter, while processing behaviour was evaluated using a laboratory internal mixer and a single-screw extruder. Strong linear correlations were observed between Mooney viscosity, RPA measurements, rheological extrusion die data, and extrusion performance. In contrast, no correlation was found with analytical measurements, Wallace plasticity, PRI, or mixing characteristics. Multimodal factor analysis confirmed these relationships and supports the use of rheological testing methods for more effective prediction of natural rubber behaviour during processing.

HYDROPHILIC SORBENTS BASED ON NATURAL POLYMERS

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The greatest use of hydrophilic sorbents (hydrogels) is in agriculture, as the soil often suffers from drought. The possible use of hydrogels can ensure access of plants to water and possible growth, and better tolerance to drought. Many hydrophilic sorbents that appear on the market are produced on the basis of fossil resources, which increases the burden on the environment. The natural polymers from which our sorbents are obtained are easily degradable. This is related to our choice of this topic; environmental protection is increasingly important. The aim was to verify whether it would be possible to produce hydrophilic sorbents from waste biomass, i.e. using raw materials that people get rid of. Synthetic hydrophilic sorbents have higher efficiency compared to our hydrophilic

sorbents, which are produced from waste biomass, but tend to be more expensive and, above all, have a negative effect in the form of the production of microplastics which are subsequently deposited in the soil. The advantage of using natural polymers is primarily a cheap and simple source, as the materials come from residues that would otherwise end up in the form of unused waste, which supports the circular economy of agricultural products. Such use of fruit and vegetable peels, plant fibers, or wood sawdust is very effective and meaningful for the renewal of the planet and supports the use of natural polymers in the spirit of a circular economy.
Acknowledgements: The contribution is funded by the project of the Czech Republic Technology Agency TS02030028.

ISOTHERMAL THERMOGRAVIMETRIC ANALYSIS AS A METHOD FOR DETERMINING THE THERMAL STABILITY OF PVC.

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Thermal degradation of poly(vinyl chloride) (PVC) is a key factor affecting its processability. Measuring thermal stability is therefore one of the key properties monitored in the evaluation of the quality of PVC. Thermogravimetric analysis (TGA) offers itself as an industrially applicable method for determining the thermal stability of PVC due to the possibility of automated measurement of a series of samples. However, its potential in the isothermal mode has not been yet systematically evaluated.
This work compares different methods for determining thermal stability of model PVC mixtures. Standardized procedures are included: the Congo red test, widely used in industrial practice, the continuous potentiometric titration, tracking hydrogen chloride release over time, and the thermogravimetric analysis in isothermal mode. The model mixtures contain various stabilizing systems commonly used in practice, specifically organotin, lead, and calcium-zinc based stabilizers, as well as plasticizers with different vapor tensions. The study evaluates the mutual correlation of the methods used and assesses the possibility of isothermal TGA as an alternative method for evaluating the thermal stability of PVC.

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NEW MEMBRANES FOR MIX GAS AND FLUE GAS SEPARATION

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Combustion technology is a significant source of industrial emissions. Along with solid waste, various compounds produced during combustion are emitted in gaseous form. Although current methods for purifying waste gases allow flue gases released into the atmosphere to meet emission standards, these technologies are approaching their maximum separation capabilities. These membranes and the overall CC technology must also address pollutants such as SO2, NOx, and HX. We aim to determine whether our new separation method can be as effective as current polymeric membranes, as evidenced by several academic studies and pilot tests by membrane producers. Developing a process that efficiently removes SO2, NOx, HX, and recovers water without necessarily removing CO2 would be advantageous, especially since CC will be feasible only at sites where further processing is possible. Therefore, there may be a demand for efficient technology without CC, which can be combined with existing flue gas purification systems, particularly on smaller scales. A unique lab-scale apparatus for testing flue gas purification has been constructed. Using the tested flat sheet membrane Toray, we achieved purification of feed gas to levels required by the European Commission's 2021 legislation. Various separation conditions (pressure above and below the membrane, separation temperature, feed and sweeping gas flux) were tested to identify optimal parameters. Our results demonstrate the high separation potential of the "water condensing membrane" for SO2 and CO2 removal from flue gas. Another approach was to use the ultrapermeable polymer of intrinsic microporosity (PIM) based on a tetramethyltetrahydronaphthalene unit coupled with bicyclic triptycene (PIM-TMN-Trip). Permeation tests with a CO2-N2-O2-SO2 mixture, simulating flue gas from power plants, were carried out using an in-house developed permeation unit. The results demonstrated very high permeability of the membrane for sulfur dioxide (SO2) and high permeability for carbon dioxide (CO2), with values primarily between the Robeson upper bound from 2008 and the more recent upper bound reported in 2019. The membrane exhibited moderately high mixed gas selectivity for SO2 and CO2 relative to N2 (21 and 11, respectively), combined with very high permeability (28·10^3 and 30·10^3 Barrer, respectively), indicating its potential for industrial gas separation processes. The SO2/CO2 mixed gas selectivity was relatively low (around 1.8), but comparable to other novel membranes, with both gases being removed simultaneously during the CO2 separation process.

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BIGUANIDE LIGAND-SUPPORTED AL/MG/ZN CATALYSTS FOR RAPID AND VERSATILE RING-OPENING POLYMERIZATION TO BIODEGRADABLE POLYESTERS AT AMBIENT-CONDITIONS

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Plastic materials synthesized by the Ring-Opening Polymerization (ROP) of various carboxylic acid derivatives, oxides and carbonates, discovered more than a century ago, have been put aside by both producers and consumers in favor of polyolefins produced from fossil fuels. The field of biodegradable polymers area was reborn with a demand to decrease the consumption of fossil sources and to reduce non-degradable solid waste such as microplastics, which contribute to marine contamination.
Their production is dominated by polylactide prepared by the solvent-free, high temperature process initiated by tin(II) octoate. Although the tin(II) compounds and complexes are supposed to be less toxic than for example pyridine, several authorities are calling for strict avoidance of heavy metals from materials used, for example, for food packaging or medicine.
As a part of our research program, we prepared and tested several aluminum, zinc and magnesium biguanide complexes in ROP. The hyperactivity of these complexes towards the ROP of several cyclic esters and trimethylene carbonate was utilized in the very rapid synthesis of sequential or statistical co-polymers, which originated also from monomers bringing contrasting properties, *ε*-CL and TMC.

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MOLECULARLY IMPRINTED POLYMERS TEMPLATED WITH STRUCTURALLY RELATED TERPENOIDS FOR SELECTIVE SEPARATION

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Molecularly imprinted polymers (MIPs) represent a promising class of functional polymeric materials capable of selective recognition of target molecules. In this study, a series of MIPs templated with structurally related terpenoids were synthesized and characterized. The selected template molecules were thymol, geraniol, α-terpineol and linalool (Figure 1), which naturally co-occur in plant extracts and exhibit similar physicochemical properties, making their separation challenging [1].

All polymers were synthesized under identical reaction conditions to enable a systematic comparison of their adsorption behavior. Corresponding non-imprinted polymer (NIP) was prepared as reference materials. The structural and textural properties of the polymers were characterized using thermogravimetric analysis, nitrogen adsorption–desorption measurements and microscopic techniques. The materials exhibited mesoporous structures typical of crosslinked polymer networks.

Adsorption performance was evaluated through kinetic binding experiments and equilibrium adsorption isotherms using the respective template molecules. The kinetic studies allowed the assessment of binding rates and equilibrium times, while isotherm analysis provided information on adsorption capacity and affinity. The applied experimental design enables systematic evaluation of the relationship between template structure and adsorption performance of the resulting polymers. In addition, the obtained data provide initial insight into selectivity trends among structurally related terpenoids.

This work provides a consistent experimental framework for comparing terpenoid-templated MIPs and contributes to the understanding of their potential application in the separation of structurally similar natural compounds.

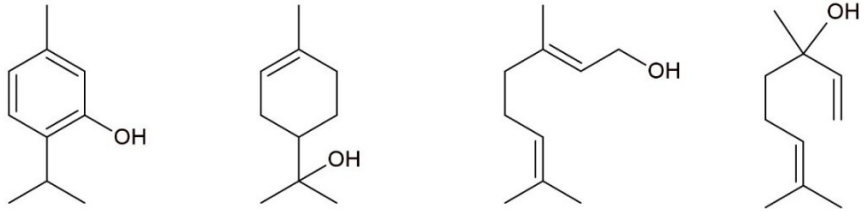

Figure 1: Chemical structures of the selected terpenoids (from left: thymol, α-terpineol, geraniol, linalool)

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DEGRADATION OF CELLULOSE FABRICS

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A significant part of the textile industry currently uses fibers made from petroleum products. However, as this industry has been a major polluter in recent years, efforts are being made to replace synthetic fibers with natural-based materials. Currently, attention is focused on regenerated cellulose – viscose, whose production using ionic liquids limits the burdening of the environment.

This work is focused on comparision of degradation behaviour of so prepared viscose in comparision with commercial polyester fibres and textiles. Accelerated aging test simulating exposure to daylight spectrum, humidity, and increased temperature was performed utilizing xenon test chambre. Degradation tests were performed also in cow manure, compost, and in abiotic aquatic environment with constant pH. The evaluation consists of monitoring changes in molar mass, color, thermal properties, chemical structure, and fiber morphology.

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PRINTED INVISIBLE MARK WITH UPCONVERSION VISUALIZER – IDENTIFICATION OF ARCHIVAL DOCUMENTS AND PROTECTION AGAINST THEFT

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When valuable items are lost, it is important to identify the owner of the item, whether it be archives, books, graphic sheets, maps, plans, or original photographs. Stamps and stickers are easy to remove, so a mark is sought that would be permanent, invisible, and resistant to restoration work.
A common solution to this problem is to mark the archived item in a way that is not obvious during normal viewing and thus escapes the attention of the thief, but allows the code to be read and the original owner to be identified if the item is recovered. The situation is somewhat similar to the protection of securities and goods against counterfeiting. However, in the case of archival and library collections, it is not only necessary to distinguish between the original and the counterfeit, but the mark on the document/book should also carry at least brief information clearly identifying the owner.
The hidden identification mark should be invisible in light, invisible in UV light, show no fluorescence or UV-induced contrast, be printable using standard printing techniques such as screen printing or pad printing, be readable/recognizable only spectroscopically, and be resistant to possible restoration interventions, mechanical abrasion, chemically non-reactive, inert to paper substrates and other cellulose fibers, and resistant to aging.
The information part of the proposed identification element contains various ratios of elements that do not occur in any paper document and can only be identified from the XRF spectrum. It is thus possible to compile a chemical code with many variants. So far, 4^4 = 256 variants of the chemical code have been verified.
The proposed invisible identification element also contains a location part used for targeting the spectrometer, as the mark is not visible. Therefore, the so-called up-

conversion phenomenon of special pigments is used, providing green fluorescence after two-photon excitation by a NIR laser.
The effect of the applied identification element on the physical and chemical properties of the paper substrate is minimal and does not manifest itself even after artificial aging tests.

Acknowledgements: The authors would like to thank the Ministry of the Interior of the Czech Republic for its support through the security research project VI20162019037, as well as all the project co-researchers.

POLYMERS AND COMPOSITES

POSTERS

RECYCLED PTFE POWDER-BASED MATERIAL FOR TRIBOLOGICAL APPLICATIONS

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Poly(tetrafluoroethylene) (PTFE) is a widely used polymer in the production of tribological elements due to its specific properties. Their production produces a large amount of chips that end up in waste, as well as any rejects or products after application. Nowadays, resource consumption is constantly increasing and waste production is growing, which is expected to double in the next three decades. Recycling waste from production would allow at least some suppression of this trend. This work is a reaction to the traditional concept of a linear economy and mass consumption, which is unsustainable in the long term. PTFE can be recycled chemically (by pyrolysis or irradiation) or mechanically. In this case, it was mechanical recycling, because PTFE is very stable and chemical recycling is very expensive. The waste from production would therefore be crushed and ground into very small particles with dimensions approaching virgin PTFE raw material and could be reused.
In this work, PTFE products intended for recycling were ground. The particle size of the resulting recycled material was measured using microscopy. Eight powder mixtures with different ratios of recycled material to the original mixture were prepared by mixing. Test specimens were prepared from the mixtures. Furthermore, several technological processing procedures (so-called resintering) were tested, the suitability of which was assessed using microscopy and tensile properties. A suitable resintering program was selected. Then, tribological and mechanical testing was carried out. Based on the test results, a mixture with a suitable ratio of recycled material/primary raw material was selected, which showed suitable utility (especially tribological) properties enabling its application in industry as well as in the case of components made from the mixture without the addition of recycled material.

INFLUENCE OF NR/BR AND SBR/BR BLENDS FORMULATION ON THE COURSE OF VULCANIZATION AND PROPERTIES OF THE VULCANIZATES

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Rubbers have been mixed for many years, both from the processing reasons, and because of requirements for the properties of the resulting rubber goods. This work deals with blends of natural rubber (NR) with butadiene rubber (BR) and styrene-butadiene rubber (SBR) with butadiene rubber, which are widely used for the manufacture of tires and technical rubber.
For each of the blends, three types of curing systems were used (standard for each rubber and sulphurless system). In these blends, the influence of formulation on the course of vulcanization and properties of the vulcanizates has been monitored. Further efforts were

made to determine whether the formation of the network common to both rubbers, i.e. mutual co-vulcanization takes place. For the characterization of rubber blends and vulcanizates, a variety of methods, such as cure-meter measurements (RPA), scanning electron microscopy (SEM) or dynamic-mechanical analysis (DMA).

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3D-PRINTED CAPSULES: AN INNOVATIVE DOSAGE FORM FOR FECAL MICROBIOTA TRANSPLANTATION

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The aim of this study was to develop and characterize capsules prepared using HME and FDM 3D-printing techniques as a novel, non-invasive approach for dysbiosis treatment. The 3D-printed capsules were designed to protect the fecal microbiota transplant (FMT) from adverse gastrointestinal conditions, particularly gastric acidity and proteolytic enzymes, and to enable its targeted release in the colon. Capsule formulations consisted of 80/90% HPMC combined with 10/20% selected natural or semi-synthetic polymers [1,2], yielding 14 tested variants. HPMC provided time-triggered release mechanism, while biopolymeric polysaccharides enabled microbiota-triggered mechanism due to the enzymatic activity of the colonic microbiota [3]. For comparison, capsules based on pH-dependent polymers were also evaluated to assess the influence of their composition on capsule properties and release behavior. The study aimed to confirm that biodegradable polysaccharide-based capsules can ensure targeted colonic delivery of FMT and potentially provide prebiotic benefits. The capsules were assessed using pharmaceutical-technology tests, including disintegration, dissolution test with pH-gradient, mechanical strength, mass and dimensional uniformity. Stability over time, interactions with the liquid filling, moisture content, and hygroscopicity were also evaluated. Based on the results, the most promising formulations underwent dissolution testing in biorelevant media and *in vivo* assessment in healthy volunteers. Capsules containing 20% gellan exhibited a lag time of approximately 8 hours, indicating successful colonic targeting, which was further supported by disintegration tests showing intact capsules after six hours. The selected formulation was additionally monitored during gastrointestinal transit in piglets, experimentally confirming the suitability of the designed dosage form and its potential for FMT administration.

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DIMETHYL CARBONATE AS PROCESSING SOLVENT FOR EXPLOSIVES

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Dimethyl carbonate is a green solvent, recommended as good alternative to acetone, ketones or cyclohexanone. It has very good solving capacity for RDX (cyclonite) and HMX (octogene) in comparison with acetone. Ir was found that some compositions prepared with the help of dimethylcarbonate and biopolymers with high explosives (RDX, HMX) offer really interesting combination of properties – low impact and friction sensitivity combined with high detonation parameters.

APPLIED CATALYSIS AND ORGANIC TECHNOLOGY

LECTURES

NANOFIBERS IN HETEROGENEOUS CATALYSIS

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Electrospinning has been widely explored and used for the synthesis of polymeric nanofibers. Its application to inorganic materials is much less common and the number of applications of nanofibrous inorganic materials in heterogeneous catalysis remains modest. Herein we have studied silica- and alumina-based catalysts exhibiting nanofibrous morphology and showed their applicability in the following examples.

First, we have prepared pure silica nanofibers and used them as support for Cu nanoparticles. It was deposited by dry impregnation technique. These materials exhibited much better copper dispersion in comparison to materials impregnated on commercial silica support (e.g., absence of CuO diffractions in XRD patterns after impregnation of up to 10 wt% Cu). Consequently, the catalytic performance of nanofibrous catalysts in ethanol dehydrogenation to acetaldehyde was better.

Second, zirconosilicate nanofibrous catalysts have been prepared in one-pot via electrospinning of silicate sol containing zirconium acetylacetonate at different conditions. Concentration of silica precursor has been identified as the decisive factor influencing the diameter of nanofibers. Consequently, the thinnest nanofibers (60 nm average diameter, SEM) exhibited the highest specific surface area, the highest number of acid sites (IR-pyridine), and the best catalytic activity in ethanol-to-butadiene conversion.

Third, one-pot electrospinning synthetic method has been applied to the synthesis of molybdenum silicate nanofibers. The band gap energies indicated that molybdenum has been homogeneously dispersed in the resulting materials. Nanofibrous molybdenum silicates have been tested as heterogeneous catalysts in propylene metathesis, exhibiting an order of magnitude higher propylene rates than catalysts prepared by dry impregnation on commercial silica support.

Finally, silica and alumina nanofibers were used as support for Cu NPs and applied in glycerol hydrogenolysis providing propylenglycol. Nanofibrous catalysts exhibited more stable catalytic performance in comparison to catalysts supported on commercial particulate materials. These examples stimulate us to explore the catalytic applications of inorganic nanofibrous materials in more detail.

RHODIUM SUPPORTED ON LAYERED AND EXFOLIATED 2D MATERIALS AS EFFICIENT CATALYSTS FOR SELECTIVE STYRENE HYDROFORMYLATION

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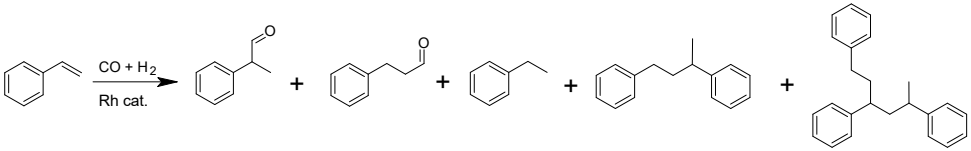
Hydroformylation is an important industrial reaction converting alkenes into aldehydes using syngas, traditionally catalyzed by homogeneous Rh-phosphine complexes that offer high activity but suffer from separation and stability limitations. Developing heterogeneous Rh catalysts with comparable performance remains challenging.
Layered and exfoliated 2D materials, including transition-metal dichalcogenides (TMDs), hexagonal boron nitride (h-BN), and delaminated 2D zeolites, represent attractive supports due to their increased surface area, tuneable electronic properties, and ability to stabilize highly dispersed Rh species. In this work, Rh catalysts supported on MoS_2, WS_2, h-BN, and selected 2D zeolites were synthesized using wet impregnation method and characterized by XRF, XRD, SEM, TEM, and N_2 physisorption. XRF confirmed successful Rh deposition, while XRD showed preservation of the layered host structures and the absence of crystalline Rh phases, indicating high dispersion. SEM and TEM analyses revealed intact morphology and well-distributed Rh nanoparticles across all 2D supports.
Catalytic performance of Rh/2D supports was evaluated in styrene hydroformylation (Scheme 1) at 100 °C and 3 MPa syngas, with Wilkinson's catalyst used as a benchmark.
Among the heterogeneous systems, Rh/h-BN exhibited the highest activity, achieving 90 % styrene conversion with aldehyde selectivity exceeding 90 %. Overall, 2D supports consistently delivered higher aldehyde selectivity than bulk 3D materials due to their strong suppression of side hydrogenation to ethylbenzene. Notably, supporting Rh on 2D materials also enabled efficient hydroformylation at lower Rh loadings (below 2 wt%) compared to their bulk counterparts.



Scheme: 1: Hydroformylation of styrene toward desired aldehydes and competing side products

Acknowledgment: This project was funded by the UCT Prague institutional support Dagmar Procházková Fund and by the Czech Science Foundation (GACR No. 23-08083M).

HIERARCHICALLY POROUS MOF-DERIVED SPHERICAL CARBON NANOCOMPOSITES WITH COBALT NANOPARTICLES FOR EFFICIENT CO_2 METHANATION

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Increasing atmospheric CO_2 concentrations, driven mainly by human activities, highlight the need for efficient strategies to mitigate emissions while supporting energy demands. Catalytic CO_2 methanation using green hydrogen offers a promising route, as it enables the production of methane, an easily stored and transported energy carrier.
This work presents a hierarchical carbon–cobalt nanocomposite catalyst derived from a cobalt-based metal–organic framework (MOF) containing a 2,6-naphthalene dicarboxylate linker.[1] The MOF is synthesized via a rapid microwave-assisted method and subsequently carbonized at 600 °C or 700 °C under argon. The resulting materials exhibit spherical morphology and contain well-dispersed cobalt nanoparticles with average diameters of 3.1 nm and 6.0 nm, respectively.
In CO_2 methanation, these CoNDC-derived catalysts achieve methane formation rates up to 10.5 $\mu mol_{CH_4}\, g_{cat}^{-1}\, s^{-1}$ at 350 °C with full selectivity toward methane. The excellent performance is attributed to the high accessibility and fine dispersion of metallic cobalt within the hierarchical carbon matrix. These findings demonstrate the strong potential of MOF-derived cobalt carbon composites as efficient catalysts for sustainable CO_2 utilization.

Acknowledgement:
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Reference

1 D. Skoda, P. Hongmanorom, B. Hanulikova, A. Dubravova, M. Cvek, I. Doroshenko, T. Pokorny, J. Varada, L. Simonikova, I. Kuritka and D. P. Debecker, *Mater. Today Chem.*, 2026, **53**, 103470.

MESOPOROUS ZEOLITE BETA FOR PRODUCTION OF LOW-EMISSION FUELS

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Efficient processing of waste lignocellulosic biomass is a key step toward decentralized production of low-emission fuels and the sustainable utilization of increasing volumes of wood waste. Biomass pyrolysis provides a liquid product rich in oxygenated compounds that requires further upgrading. This makes heterogeneous catalysts with acid sites—particularly zeolites with enhanced accessibility of active sites—highly relevant. Among them, mesoporous Beta zeolite prepared by the Hot Water Treatment (HWT) method shows exceptional potential. HWT is an environmentally friendly procedure that uses only hot water—without any organic or inorganic agents—to generate secondary porosity while preserving the crystalline BEA framework. The method has been successfully validated from laboratory to pilot and semi-industrial scale, including the preparation of semi-industrial-scale HWT Beta in a 50 L autoclave.

HWT modification resulted in a 12–15% increase in mesopore volume, a higher total pore volume, and full preservation of the acid sites required for cracking reactions. The increase in mesopore volume was further confirmed by a clear decrease in bulk density, demonstrating the formation of additional pore space and enhanced hierarchical porosity. Complementary ^{27}Al MAS NMR characterization confirmed that HWT does not disrupt framework Al, maintaining both its distribution and the catalyst's acidic functionality.

Shaping these materials into extrudates with 20% alumina enabled their use in the ex-situ catalytic stage of biomass pyrolysis.

Pyrolysis of wood chips without a catalyst produced liquids with a very high boiling point (508 °C) and a high content of aromatics. The addition of CaO in situ significantly reduced the maximum boiling point to ~293 °C but simultaneously increased the aromatic fraction. The most favorable results were achieved with the combined CaO in-situ and HWT Beta ex-situ configuration, which maintained the same boiling temperature while providing a higher yield of olefins and other valuable products.

SCALABLE MECHANOCHEMICAL PRODUCTION OF NI-CO SULFIDES FOR ALKALINE WATER SPLITTING

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Water electrolysis relies on the electrochemical splitting of water into hydrogen and oxygen, with efficiency largely determined by the activity and stability of electrocatalysts driving the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode. For large-scale hydrogen production via water electrolysis, the development of efficient, abundant, and fast and easily manufactured catalysts is crucial.

In this work, we explore a rapid and environmentally friendly mechanochemical synthesis approach to produce transition metal sulfide catalysts. This method allows the direct formation of Ni-Co sulfide materials from elemental precursors within seconds, without the need for high-temperature treatments or solvent-based processing. Consequently, the process significantly reduces the carbon footprint of the manufacturing cycle, fulfilling the strict criteria for sustainable green chemistry.

By adjusting the Ni-to-Co ratio, different compositions with distinct catalytic properties were obtained. The optimized ternary sulfide system demonstrated the highest hydrogen evolution activity in alkaline conditions, showing low overpotential, excellent stability, and long-term performance. The enhanced activity is attributed to the synergistic interaction of multiple sulfide phases and optimized metal ratios, which improve surface area, electronic conductivity, and the balance between water dissociation and hydrogen adsorption steps.

This combination of rapid, scalable synthesis, eco-friendly processing and strong catalytic performance highlights the potential of these materials for practical application in cost-effective alkaline water electrolyzers.

ACKNOWLEDGMENT

This work was funded by the EU Next Generation EU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00109, the Slovak Research and Development Agency No. APVV-24-0353, The Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No: 451-03-136/2025-03/200026), and the Science Fund of the Republic of Serbia, Program PRISMA, Grant No. 5354, Multifunctional visible-light-responsive inorganic-organic hybrids for efficient hydrogen production and disinfection-HYDIS.

MAXIMIZING REFINERY PROFITABILITY THROUGH RESIDUE HYDROCRACKING

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Chevron Lummus Global, The Hague, The Netherlands

Refiners worldwide are showing renewed interest in **heavy oil upgrading** as several major residue-processing projects have recently come online, with more scheduled in the near future. As the industry increasingly turns to lower-cost, heavier crudes with higher contaminant levels, advanced bottom-of-the-barrel upgrading technology have become essential for meeting tightening product specifications and maximizing refinery profitability. CLG highlights that refiners have more **economically attractive options** for residue disposition than traditional LSFO or RFCC feed pathways.

Residue hydrocracking has progressed significantly, with achievable vacuum residue conversion increasing from 60–80% to 80–90% and beyond; along with increased commercially proven on-stream factors. These advancements allow refiners to **minimize low-value product streams** while maximizing production of **clean transportation fuels** and **petrochemical feedstocks**.

This presentation will summarize major technological developments enabling this performance step-change - including breakthroughs in detailed resid characterization, catalyst and catalyst-system innovation, and optimized process design and operating strategies. Together, these advances provide refiners with a **robust suite of high-reliability, high-conversion solutions** for economically upgrading the heaviest refinery streams.

We will review recent performance results from CLG's **LC-FINING** and **LC-MAX** technologies, as well as the extension of slurry-phase residue upgrading through CLG's **LC-SLURRY** technology. Additionally, we will discuss the continued progress of the **CLG–Eni Alliance** formed in 2021 to commercialize the **Eni EST** process. Collectively, these technologies offer refiners **flexible pathways** to increase conversion, reduce unconverted oil, and meet growing demand for both clean fuels and petrochemical feedstocks.

CATALYTIC DISTILLATION: A NEW ERA FOR DME PRODUCTION

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Lummus Technology, The Hague, The Netherlands

The production of Dimethyl Ether (DME) represents a key pathway towards a sustainable energy future. However, conventional DME production processes are typically inefficient, energy-intensive, and environmentally burdensome. This presentation introduces an advanced design and an efficient alternative to produce DME: integration of catalytic distillation, a highly intensified technology that combines chemical reaction and separation in a single step, while significantly reducing energy consumption and capital costs.

Our approach focuses on developing and optimizing innovative reactor configurations, advanced catalyst systems, and efficient separation strategies to minimize energy losses and environmental impact. The outcome is a scalable, cost-effective, and environmentally friendly DME production process, suitable for deployment into any new and existing industrial infrastructure.
This breakthrough technology has the potential to reshape the energy landscape by enabling the widespread adoption of DME as a clean and sustainable energy carrier.

Quantitative Double-Tilt Tomography and HR-TEM for the Structural Characterisation OF PHOTOCATALYSTS AU/TIO_2 RASPBERRY-COLLOID INVERSE OPALS

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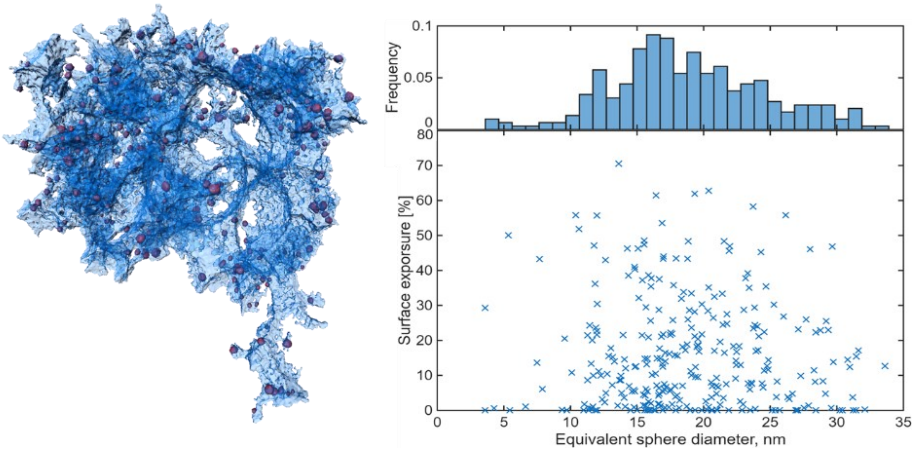
The performance of Au/TiO_2-based photocatalysts in the reverse water–gas shift reaction is linked to the embedding of nanoparticles (NPs) and strong metal–support interactions (SMSI). However, the precise quantification of NPs embedding and SMSI within complex, hierarchical supports, such as raspberry-colloid-templated inverse opals (RC-IOs), remains a significant challenge for standard 2D imaging.
This study demonstrates the power of double-tilt electron tomography (ET) combined with double aberration-corrected TEM to resolve the ordered structures of RC-IOs. By utilising a dual-axis tilt series and refined alignment protocols in IMOD,3D volumes of the RC-IOs were reconstructed with high-precision. This approach enables the 3D quantification of Au nanoparticle embedding depth and spatial distribution within the TiO_2 support, bypassing the artefacts common in single-axis reconstructions of porous materials.
Our high-resolution analysis further explores the structural evolution of the Au-TiO_2 interface after reductive and oxidative treatment. Using aberration-corrected TEM imaging, we directly observe the induction of reversible SMSI, where the encapsulation of Au NPs are correlated with photocatalytic testing. These results provide a robust structural basis for understanding the stability and catalytic activity of Au/TiO_2 RC-IOs, highlighting the necessity of multi-dimensional electron microscopy in the design of next-generation photocatalysts.



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This work was supported by a Science for Sustainability grant from Utrecht University. Electron tomography and HR-TEM work was performed in the Electron Microscopy Center at Utrecht University.

CO_2 CYCLOADDITION TO STYRENE OXIDE OVER MCM-41/CTAB

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The catalytic cycloaddition of carbon dioxide to epoxides represents a sustainable route for the utilization of CO_2 as an abundant C_1 building block and an environmentally benign alternative to conventional phosgene-based carbonate synthesis. However, due to the thermodynamic stability and kinetic inertness of CO_2, efficient catalytic systems are required to achieve high conversion and selectivity under practical conditions.
This contribution focuses on the cycloaddition of CO_2 to styrene oxide (Fig. 1) employing a mesoporous silica-based catalytic system MCM-41/CTAB. MCM-41 provides a high specific surface area and uniform pore structure, while hexadecyltrimethylammonium bromide (CTAB) acts as a source of bromide anions capable of promoting epoxide ring opening.
Reactions were performed in a stainless-steel autoclave at 120 °C and 1.2 MPa. The influence of reaction parameters was systematically investigated, including the comparison of homogeneous and heterogeneous catalysis, as well as the evaluation of different heterogeneous silica-based materials. The effect of various co-catalysts, solvents, catalyst loading and catalyst reusability was also examined. Reaction products

were analyzed by GC-MS, and the catalysts were characterized using UV-Vis and FTIR spectroscopy, elemental analysis and nitrogen physisorption.
Among the tested systems, potassium iodide (KI) was identified as the most effective co-catalyst. The highest conversion of styrene oxide (100 %) was achieved in 1-methyl-2-pyrrolidone using 75 wt% MCM-41/CTAB in the presence of 0.1 mmol KI. The highest selectivity towards styrene carbonate (84 %) was obtained in *N*,*N* dimethylformamide employing 25 wt% of the impregnated catalyst MCM-41/$CTAB_i$ without the addition of KI. The results demonstrate that silica-based materials containing quaternary ammonium species represent promising heterogeneous systems for efficient CO_2 cycloaddition to styrene oxide.

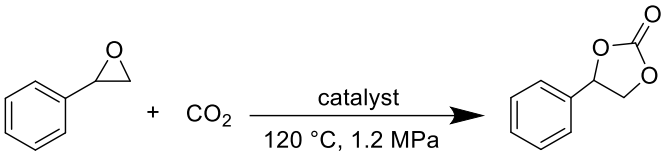

Figure 1: Cycloaddition of CO to styrene oxide

This work was supported from the grant of Specific university research – grant A1_FCHT_2026_003

SYNTHESIS OF CARVYL ACETATE BY ONE-POT REACTION

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α-Pinene oxide is a valuable starting material for synthesizing a wide range of fine chemicals, notably for perfumery and pharmaceuticals. Its reaction with acetic anhydride, catalyzed by an acid, proceeds in a one-pot, two-step sequence: isomerization to monoterpenic alcohols followed by their acetylation. This approach to the synthesis of monoterpenic acetates has been only marginally investigated. Štekrová et al. [1] used β-pinene oxide as the substrate in a reaction catalyzed by montmorillonite K10, which afforded perillyl acetate as the main product, accompanied by minor product myrtenyl acetate. Tatarova et al. [2] studied α-pinene oxide reactivity and obtained traces of acetates without additional solvent. Several studies on the isomerization of α-pinene oxide have reported that the use of basic solvents enhanced formation of monoterpenic alcohols [3]. In this study, we present the selective synthesis of carvyl acetate from α-pinene oxide. Carvyl acetate is a flavoring agent with a sweet, mint-like aroma and may also be used in dental hygiene applications. [4]. In this study, zeolite H-Beta 25 was selected as the heterogeneous catalyst. We optimized the reaction conditions by varying catalyst loading, solvent type and volume, reactant ratio, and temperature. Based on our studies of monoterpenic oxide isomerization and alcohol acetylation, the highest isolated

yield of carvyl acetate (47%) was obtained using 20 wt% zeolite H-Beta 25 as catalyst, with α-pinene oxide:acetic anhydride:*N,N*-dimethylformamide molar ratio of 1:8:8, , at 90 °C for 4 h. The main by-product was campholenic aldehyde, obtained in 25% yield, which constitutes an important precursor for the synthesis of compounds exhibiting sandalwood-like scent. This work deepens understanding of the reaction between α-pinene oxide and acetic anhydride and establishes a novel synthetic route to carvyl acetate.

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Evaluace netradičních odpadních surovin pokročilými recyklačními technologiemi. Nový přístup k recyklaci pneumatik .

Termochemická recyklace pneumatik představuje jednu z nejperspektivnějších technologií pro ekologické a ekonomicky efektivní nakládání s odpadními pneumatikami.

Doc. Dr. Ing. Kuráň Pavel, UJEP Ústi nad Labem
Doc. RNDr. Bačiak Miloslav,Ph.Dr ,UJEP Ústi nad Labem
Mgr. Pátek Jaroslav MBA, UJEP Ústi nad Labem

GLYCEROL VALORIZATION INTO HIGHER VALUE-ADDED PRODUCTS: PRODUCTION OF BIO 1,2-PROPANDIOL

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University of chemistry and technology, Prague

Introduction:

Glycerol is a major by-product of biodiesel production, with about 100 kg generated per 1 ton of biodiesel. The increasing biodiesel output results in a glycerol surplus, creating a need for efficient valorization. A promising route is its conversion to 1,2-propanediol (1,2-PDOL), an important chemical used in polyester resins, plastics, coatings, and in food, cosmetic, and pharmaceutical applications.

Methodology:

Glycerol hydrogenolysis was investigated both in gas and liquid phase. Gas-phase experiments were conducted in a glass tubular flow reactor using Cu-based catalysts, while liquid-phase reactions were performed in an autoclave under elevated hydrogen pressure. The effects of temperature, pressure, catalyst loading, and feed composition on conversion and selectivity were systematically studied. The chemical equilibrium of the

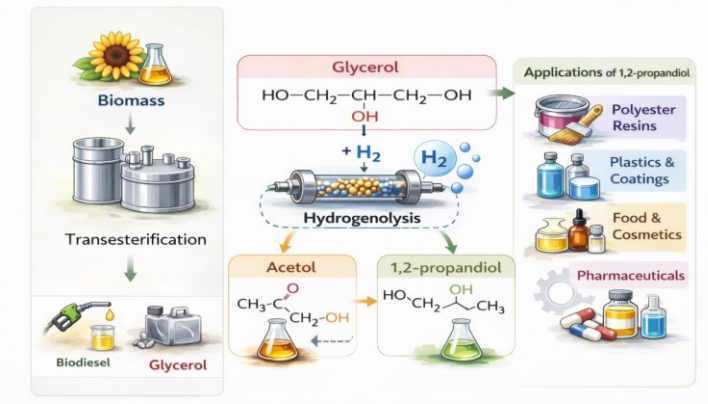
acetol–1,2-PDOL system was experimentally determined in a metal reactor with direct GC injection and used for process modeling in Aspen Plus.

Results:

Higher temperature increased glycerol conversion but also promoted by-product formation. Cu-based catalysts showed limited activity in the gas phase, whereas a nickel catalyst exhibited superior performance. The experimentally determined acetol–1,2-PDOL equilibrium enabled realistic process simulation.

Conclusion:

Glycerol hydrogenolysis strongly depends on operating conditions and catalyst type. Nickel catalysts proved more suitable than Cu-based catalysts under the studied conditions. The obtained data will be used for the economic evaluation of the industrial process aplication.



APPLIED CATALYSIS AND ORGANIC TECHNOLOGY

POSTERS

ADVANCED CHEMICAL DEPOSITION FOR ATOMICALLY PRECISE NANOFABRICATION OF PLATINUM CLUSTERS ON LOW-DIMENSIONAL MATERIALS

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Low-dimensional (LD) materials have gained enormous attention in catalysis due to their high activity and large surface area. While graphene and its derivatives have been widely studied, non-carbon LD materials such as transition metal dichalcogenides (TMDs) and transition metal phosphorus trichalcogenides (TMPTs) also demonstrate strong potential for catalytic applications. TMDs and TMPTs offer large surface area and many edge sites, which are good for anchoring metal nanoparticles, making them particularly attractive as support for developing advanced heterogeneous systems. Moreover, the layered morphology of these materials enables the intercalation of foreign atoms between layers, which can modify catalytic behaviour through enhanced metal-support interactions. Such interactions play a crucial role in determining catalytic performance, including activity, selectivity, and stability.
Platinum (Pt) is among the most effective catalytically active metals; however, its high cost requires strategies to maximize its efficiency while minimizing utilization. The deposition of Pt nanoparticles onto support materials is the most common approach to improve its dispersion and enhance catalytic activity.
Atomic layer deposition (ALD) is an advanced chemical deposition technique, which enables the fabrication of ultra-small, uniformly distributed metal clusters with atomic precision and strong metal-support interaction at the substrate's reactive sites, owing to its unique deposition chemistries and interfacial energies. ALD enables precise control over metal loading and dispersion, which ensures uniform distribution of metal atoms across the support while preventing agglomeration.
This study aims to utilize the advanced ALD technique to fabricate Pt clusters on LD materials (TMDs, TMPTs) and to investigate the specific interactions between Pt clusters and their supports.

This work was supported by the Czech Science Foundation (GACR No. 23-08083M) and Specific University Research – UCT Prague Rector's Junior Grant (JIGA 2026)

IN SITU DRIFTS STUDY OF CO ADSORPTION OVER PLATINUM AND COPPER SUPPORTED ON 2D MATERIALS

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Carbon monoxide (CO) is widely used as a probe molecule in infrared spectroscopy for the characterization of surface metal sites. The stretching frequency ν(CO) of adsorbed CO is

influenced by several factors, including the nature of the metal sites (e.g., coordination number and oxidation state), the adsorption mode of CO, and lateral interactions between adsorbed CO molecule, commonly referred to as dipole–dipole coupling. Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) enables the investigation of CO adsorption under *in situ* conditions and allows the determination of different adsorption sites on supported metal surfaces.
Graphene oxide (GO) and molybdenum disulfide (MoS_2) are promising catalyst supports due to their unique structural and electronic properties, which can affect the dispersion of metal nanoparticles and their interaction with the support. In this work, Pt- and Cu-based catalysts supported on these two-dimensional (2D) materials were prepared by wet impregnation followed by chemical reduction, with metal loadings of 2 and 10 wt.%. The structural and morphological properties of the prepared materials were characterized using scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM-EDS), atomic force microscopy (AFM), X-ray diffraction (XRD), and Raman spectroscopy.
In situ DRIFTS measurements were performed using a Praying Mantis™ High Temperature Reaction Chamber (Harrick Scientific) to investigate CO adsorption on the prepared catalysts and to identify the corresponding infrared bands associated with different adsorption modes. Particular attention was devoted to the assignment of the observed v(CO) bands to specific adsorption sites on the metal surface. The obtained spectra were compared the evaluate the influence of metal (Pt and Cu), metal loading (2 and 10 wt. %), and the 2D support (GO and MoS_2) on the adsorption behavior of CO.

This project was supported by the Czech Science Foundation (GACR No. 23-08083M).

A COMPARATIVE EVALUATION OF CO VS. CO_2 FEEDSTOCKS FOR SUSTAINABLE CATALYTIC METHANOL SYNTHESIS

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This research supports Europe's energy independence by creating methanol from atmospheric CO_2 and green H_2. This process turns irregular solar power into a stable liquid fuel. By capturing carbon directly, it cuts greenhouse gas emissions more than importing fossil fuels. This study compares this CO_2 method against standard CO-based production. While using CO_2 is more difficult, it is better for a circular carbon economy.
This study evaluated novel Cu-based catalysts for MeOH synthesis using a lab-scale fixed-bed reactor. Following surface activation, synthesis was performed across various temperatures to benchmark CO_2 hydrogenation against traditional CO-based pathways, specifically comparing catalytic activity and selectivity between the two carbon sources.

Performance was validated using a 4 g catalyst loading, with product mass determined via gravimetric analysis. Aqueous byproduct concentrations were quantified through Karl-Fischer titration to isolate hydrocarbon mass, enabling precise calculations of conversion and selectivity. These metrics provided a direct performance comparison between CO_2 and CO-based synthesis, benchmarking the catalyst's activity across both feedstocks.
The results reveal a significant performance gap between the two feedstocks: the CO-based pathway demonstrated high efficiency with an average yield of 24.72 %, whereas the CO_2 pathway achieved a yield of 3.32 %. While the CO-based route remains more economically viable at present due to superior material utilization, the CO_2 pathway offers a superior environmental profile by valorizing captured emissions. These findings quantify the current efficiency trade-offs in green methanol production and highlight the critical need for further catalytic optimization to bridge the gap toward a sustainable carbon economy.

3D PRINTED TABLETS IN THE CONTEXT OF PERSONALIZED MEDICINE: NEW SULFONAMIDES AS POTENTIAL DRUGS FOR ALZHEIMER'S DISEASE INCORPORATED INTO DELIVERY SYSTEM VIA PHARMACEUTICAL 3D-PRINTING

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The use of hot melt extrusion combined with fused deposition modeling 3D printing was explored to enhance the solubility and bioavailability of poorly water-soluble compounds intended for Alzheimer's disease (AD) therapy.[1] AD, a neurodegenerative disorder with no definitive treatment, affects millions worldwide, underscoring the urgent need for effective and personalized therapeutic strategies.[2,3] Four sulfonamide-derived compounds, identified as potential AD therapeutics, were synthesized and successfully incorporated (loads between 10 – 50 wt.%) into customized, 3D-printed oral dosage forms. These 3D-printed tablets were evaluated for properties such as hardness, thermo-analytical characterization, dissolution, cytotoxicity, and stability. Notably, successful amorphization of the incorporated APIs was observed in most 3D-printed tablets, which may be critical for improving solubility. *In vitro* dissolution testing revealed multiple favorable release profiles, with several formulations demonstrating sustained or enhanced drug release suitable for the therapeutic requirements of AD. When compared to the dissolution data of the corresponding conventional matrix tablets, the present 3D-printed tablets offered superior or comparable dissolution characteristics, demonstrating the potential of the personalized medicine and remote digital control for optimizing patient-specific treatments.

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TRANSITION METAL DICHALCOGENIDES (TMDS) SUPPORTED RHODIUM CATALYSTS FOR ENHANCED HYDROFORMYLATION ACTIVITY AND SELECTIVITY

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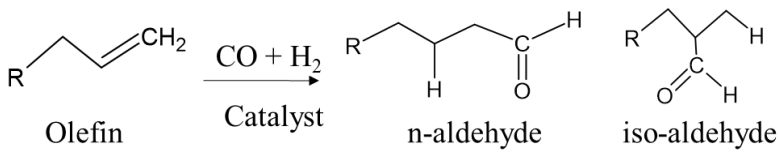
Hydroformylation is the addition of synthesis gas (syngas), a mixture of carbon monoxide (CO) and hydrogen (H_2), to olefins in the presence of a catalyst to form aldehydes. In this atom-economic transformation, a hydrogen atom and a formyl group (H–C═O) are introduced across the carbon–carbon double bond, yielding linear and branched aldehydes as shown in **(Scheme 1)**. Its continued reliance on homogeneous rhodium-based catalysts presents challenges related to catalyst separation, recyclability, and sustainability. This study aims to develop and investigate heterogeneous hydroformylation catalysts based on rhodium nanoparticles supported on transition metal dichalcogenides (TMDs) in their bulk and exfoliated form. Two-dimensional TMDs materials were prepared via high-pressure homogenization exfoliation and employed as supports for rhodium using wet impregnation methods. Comprehensive physicochemical characterization was performed to elucidate metal dispersion, structure, and metal support interactions. Catalytic performance was evaluated in batch hydroformylation reactions under syngas conditions using a structurally and electronically diverse range of olefin substrates, including linear aliphatic, aromatic and cyclic olefins. Particular emphasis was placed on correlating substrate structures with hydroformylation activity of prepared catalysts. This work provide fundamental insights into structure performance relationships in transition metal dichalcogenides–supported hydroformylation catalysts and to establish a foundation for more sustainable and efficient alternatives to conventional homogeneous catalytic systems.



Scheme: 1: General reaction scheme of hydroformylation reaction

Acknowledgment: This work was supported from the grant of Specific university research – grant No A2_FCHT_2026_053.

CATALYTIC ACTIVITY DISTRIBUTION OF INDIVIDUAL CATALYST PARTICLES IN ONE CATALYST BATCH

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Hydrotalcites (layered double hydroxides, LDHs) are widely used as heterogeneous base catalysts, where catalytic performance strongly depends on the distribution and strength of basic sites. Conventional catalytic tests provide only average activity of a catalyst batch and do not reveal possible inter-particle heterogeneity, which may significantly influence reaction selectivity and stability.

In this work, the catalytic activity of individual hydrotalcite particles was investigated using a single-particle fluorescence labeling approach. The method is based on the base-catalyzed disproportionation of furfural, where the reaction product undergoes subsequent polymerization, forming fluorescent species inside catalytically active particles. The fluorescence intensity of individual particles is therefore proportional to their catalytic activity and allows direct visualization of activity distribution within one catalyst batch.

Two hydrotalcite samples with different Mg/Al ratios were studied together with several pretreatment procedures, including calcination and hydration, which modify the structure and the distribution of basic sites. Individual particles were analyzed by correlative fluorescence microscopy and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDS), enabling correlation between catalytic activity and elemental composition of the same particle. Special attention was devoted to the influence of EDS acquisition parameters and data processing workflow on the reliability of Mg/Al ratio determination.

The results show a significant variability of catalytic activity among individual particles within a single catalyst batch. Hydrated samples exhibit substantially higher activity compared to calcined samples, indicating the importance of weak basic sites formed after structural reconstruction. For some samples, catalytic activity increases with Mg/Al ratio, while at higher Mg contents the activity reaches a plateau, suggesting the existence of an optimal composition.

The presented methodology allows direct structure–activity correlation at the level of individual catalyst particles and provides insights that cannot be obtained from conventional bulk catalytic measurements. This approach represents a powerful tool for understanding heterogeneity in heterogeneous catalysts and for rational optimization of hydrotalcite-based catalytic materials.

This project was supported by the Czech Science Foundation (GACR No. 23-08083M).

PREPARATION OF NON-SYMMETRIC ETHERS OF 2-PHENYLETHANOL BY DIRECT DEHYDRATION

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Ethers of 2-phenylethanol are attractive targets because they combine the characteristic reactivity of benzylic systems with enhanced stability and tunable lipophilicity, making them valuable intermediates in organic synthesis and fragrance chemistry [1,2]. Their structural variability further enables precise control over volatility and sensory properties, which is beneficial for designing novel aroma compounds and related functional materials. Among these derivatives, the most prominent is the ether formed with isoamyl alcohol, commercially known as Anther® (Fig. 1).

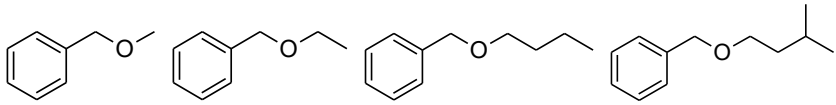

Fig. 1: Ethers of 2-phenylethanol (methyl-, ethyl-, butyl-, isoamyl- = Anther®)

These non-symmetric ethers are typically prepared by dehydration of the corresponding alcohols, a transformation commonly catalyzed by strong mineral acids, most often sulfuric acid. The present work focuses on the acid-catalyzed etherification of lower alcohols (methanol, ethanol, butanol, and isoamyl alcohol) with 2-phenylethanol carried out in several reaction arrangements, evaluating how different setups and reaction conditions influence ether formation and overall process efficiency. The highest conversion of 2-phenylethanol was achieved using a Dean–Stark apparatus using sulfuric acid as catalyst, where continuous removal of water shifted the equilibrium toward ether production. When *n*-butanol reacted with 2-pehylethanol, *t*-butyl 2-phenylethyl ether was the predominant product due to extensive isomerization, while in the case of isoamyl alcohol the extent of isomerization was significantly lower. These findings provide valuable insight into how reaction environment, alcohol structure, and catalytic conditions govern the efficiency and selectivity of acid-catalyzed etherification of 2-phenylethanol.

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PROCESS ENGINEERING

LECTURES

SUSTAINABILITY TRENDS AND THE DECARBONISATION IN THE PLASTIC INDUSTRY SUPPLY CHAIN

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The plastics industry is undergoing a profound transformation driven by sustainability requirements, decarbonisation targets, and evolving regulatory frameworks such as CSRD, the GHG Protocol, Environmental Product Declarations (EPD), and the Product Environmental Footprint (PEF). This lecture examines key sustainability trends in the plastics industry, with a focus on decarbonization across the entire supply chain, from raw material extraction and polymer production to processing, logistics, use, and end-of-life management, including recycling. A central theme is the role of Life Cycle Assessment (LCA) as a quantitative, life cycle–based methodology for identifying environmental hotspots and supporting informed decision-making. The lecture highlights the differences and complementarities between product-level LCA and organisational carbon footprinting, particularly the limitations of aggregated Scope 3 data for product-oriented strategies. Practical examples from the plastics value chain illustrate how LCA can support material optimisation, recycling strategies, and realistic decarbonisation pathways at product, organisational, and sectoral levels.

TECHNICKO-INŽENÝRSKÁ PŘÍPRAVA PILOTNÍCH PROJEKTŮ CCS A CCU V ČESKÉ REPUBLICE (2026–2027)
Integrovaný přístup k budování národního systému Industrial Carbon Management

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Evropská unie vstoupila do fáze reálného nasazení technologií zachytávání, využití a ukládání CO_2 (CCUS). V návaznosti na Industrial Carbon Management Strategy a cíle Net-Zero Industry Act, které stanovují minimální injekční kapacitu 50 Mt CO_2 ročně do roku 2030, přechází diskuse od koncepčních dokumentů k praktické přípravě konkrétních projektů. Česká republika na tento vývoj reaguje prostřednictvím Akčního plánu rozvoje CCUS (2025–2030), jenž vymezuje sektory, objemy a institucionální rámec pro budování národního systému řízení uhlíku.
Příspěvek představuje koncepci a aktuální stav technicko-inženýrské přípravy prvních pilotních projektů CCS a CCU v ČR realizovaných v letech 2026–2027 v rámci platformy CO2 Czech Solution Group (CO2CZ). Projekt je strukturován jako integrovaná příprava celého hodnotového řetězce – od záchytu CO_2 u průmyslových emitentů (chemie, cement, vápno, ocel) přes úpravu, kompresi a variantní scénáře přepravy (železnice / potrubí / hybrid) až po geologické ukládání a navazující využití CO_2 v chemických a energetických aplikacích (CCU).

Hlavním cílem není realizace zařízení, ale dosažení úrovně pre-FEED / FEED-0 (v případě referenčního CCU pilotu až Basic Design), která umožní po roce 2027 plynulý přechod do investiční fáze a využití evropských a národních finančních nástrojů (Innovation Fund, Horizon Europe, Modernizační fond). Příspěvek detailně popisuje sjednocený Design Basis, metodiku multi-emitentního řešení, integraci CCS a CCU do jednoho systému Industrial Carbon Management, ekonomické hodnocení (CAPEX/OPEX, jednotkové náklady €/t CO_2) i regulatorní a bezpečnostní rámec v českých podmínkách.
Zvláštní důraz je kladen na institucionální model spolupráce průmyslu, infrastruktury, geologických autorit a státní správy a na vytvoření replikovatelného rámce, který může sloužit jako referenční model pro další středoevropské země bez přímého přístupu k offshore úložištím. Prezentace nabídne nejen technický přehled připravovaných pilotních projektů, ale i systémový pohled na to, jak transformovat strategii dekarbonizace do konkrétní, ekonomicky a regulatorně proveditelné projektové přípravy.

PRINCIPY GEOLOGICKÉHO UKLÁDÁNÍ UHLÍKU A JEHO MOŽNÉ UPLATNĚNÍ V ČR

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Geological CO2 storage is part of the set of CCUS (carbon capture, utilization and storage) technologies, designed as one of the pathways within the EU's climate neutrality commitments. The Czech Geological Survey has been engaged in research in this area within European cooperation for more than 20 years.
Geological CO2 storage requires the existence of sufficiently thick sedimentary strata with suitable physical parameters and proven traps for the permanent storage of CO2 in the supercritical phase. Among the geological units of the Czech Republic, the Vienna Basin, the southeastern slopes of the Bohemian Massif, and the Carpathian Foredeep are considered promising, both within exploited hydrocarbon deposits and in deeply buried strata primarily saturated with saline formation water. Several promising areas have already been identified, and the next steps will focus on their targeted study, including conducting pilot tests.
The preparation of a repository is a time-consuming and financially demanding process that requires compliance with legislative requirements, particularly regarding the extent of geological and geophysical surveys and modeling, along with the preparation of monitoring plans for all stages of operation. In general, it can be expected that prepared repositories in southeastern Moravia will be a suitable domestic complement to the planned strategy of exporting captured CO2 to foreign CO2 repositories.

POTENCIÁL A PILOTNÍ OVĚŘOVÁNÍ UKLÁDÁNÍ CO2 V GEOLOGICKÝCH STRUKTURÁCH ČESKÉ REPUBLIKY

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Ukládání oxidu uhličitého (CCS) představuje významný nástroj pro snižování emisí skleníkových plynů, zejména v průmyslových odvětvích s omezenými možnostmi dekarbonizace. V České republice byly identifikovány geologické struktury vhodné pro bezpečné a dlouhodobé ukládání CO2, především v oblasti jižní Moravy, severozápadních Čech a severní Moravy. Tyto struktury zahrnují jak dotěžovaná ložiska ropy a zemního plynu s relativně omezenou kapacitou, tak zejména hluboké slané akvifery, které nabízejí vyšší úložný potenciál, avšak s nižší mírou prozkoumanosti.
Celkový potenciál ukládání CO2 je omezený a jeho přesné stanovení vyžaduje komplexní průzkum. Ten zahrnuje pokročilé geofyzikální metody, zejména 3D seismická měření, realizaci průzkumných vrtů, odběr a laboratorní analýzy horninových vzorků. Součástí je také geologické modelování, simulace chování CO2 v horninovém prostředí a hodnocení geochemických a geomechanických procesů. Nedílnou součástí je rovněž posouzení rizik a návrh monitorovacích systémů pro zajištění dlouhodobé integrity úložišť.
Společnost MND je v oblasti ukládání CO2 dlouhodobě aktivní a disponuje zkušenostmi z řady výzkumných i přípravných komerčních projektů. Klíčovým krokem k praktickému využití CCS je realizace pilotních a demonstračních projektů, které by umožnily ověřit ukládání CO2 v reálných podmínkách. Tyto projekty cílí na získání zásadních data pro validaci modelů, ověření injektivity horninového prostředí, práci s reálnými vzorky a zpřesnění odhadů úložných kapacit. Zároveň přispívají ke snížení technických, ekonomických i regulatorních nejistot a k posunu technologické připravenosti směrem k předkomerční fázi.
Rozvoj CCS v České republice tak představuje důležitý předpoklad pro budování domácí infrastruktury, posílení energetické bezpečnosti a dosažení klimatických cílů při zachování konkurenceschopnosti průmyslu.

DEVELOPMENT OF CROSS-BORDER INFRASTRUCTURE FOR CARBON DIOXIDE TRANSPORT IN THE CZECH REPUBLIC

J. Mazač (Prague)

Rozvoj přeshraniční infrastruktury pro přepravu oxidu uhličitého (CO2) představuje klíčový předpoklad pro efektivní nasazení technologií zachytávání, využívání a ukládání CO2. V situacích, kdy není možné zachycený CO2 využít přímo v místě vzniku, je nezbytné zajistit jeho transport k průmyslovému využití nebo k trvalému uložení ve vhodných geologických strukturách. Rostoucí význam přeshraniční přepravy je podmíněn zejména omezenými kapacitami domácích ložisek určených k ukládání, což zdůrazňuje potřebu mezinárodní spolupráce a budování regionálně propojené infrastruktury. Vytvoření robustní evropské

sítě pro přepravu CO2 bude zásadní pro dosažení klimatických cílů a dlouhodobý rozvoj CCUS technologií. Prezentace se zaměří na koncept přepravy CO2 v České republice a na související technicko-ekonomické parametry.

ACCURATE DESCRIPTION OF THERMODYNAMIC PROPERTIES AND PHASE BEHAVIOR OF CO_2 STREAMS NECESSARY FOR DESIGN OF CCUS TECHNOLOGIES

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The design and reliable operation of CCUS (carbon capture utilization, or storage) technologies set new demands on the accurate description of the thermodynamic properties, phase equilibria, and phase transitions of CO_2-rich fluid systems. CO_2 streams will always contain impurities depending on the source of emissions and the capture technology. Admixtures such as H_2O, NO_x, SO_x, or non-condensable gases like N_2 and Ar shift the temperature and pressure phase equilibria, can react and accumulate in the form of corrosive aqueous phases, or can result in the formation of gas hydrates and other solids that block the CO_2 flow (see figure). Our team is involved in broader international research describing the thermodynamic properties and phase behavior of CO_2-rich mixtures. The theoretical work employes the multiparameter equations of state for fluid phases in combination with a physically-sound model of gas hydrates. Phase interfaces and nucleation, i.e. the initiation of new phase formation (droplets, crystals), are studied using nucleation theories such as CNT (classical nucleation theory) and DGT (density gradient theory). As part of our experimental work, the expansion chambers for the investigation of phase transition kinetics during sudden pressure drop are being developed. Members of our team are also involved in the preparation of technical standards on the impurity limits for CO_2 pipeline transport (DVGW C 260 and CEN/TC 474).

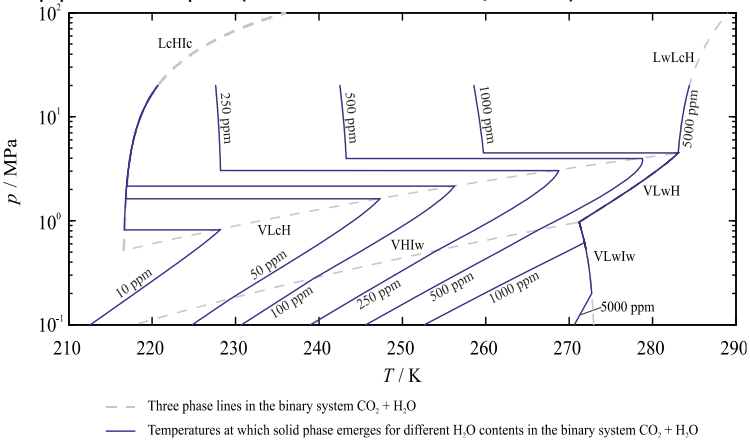

Fig.: *p, T* diagram of CO_2 + H_2O system showing conditions of the solid phase formation, i.e. water ice Iw, dry ice Ic, and gas hydrates H, depending on water content in ppm (particle per million); blue solid lines – conditions at which the solid phases form by decreasing temperature at a given pressure, gray dashed lines – three phase equilibrium lines in the binary CO_2 + H_2O mixture.

INTERREGIONAL COMPARISON OF CARBON CAPTURE, UTILIZATION, AND STORAGE (CCUS) FOR CARBON NEUTRALITY: A CASE STUDY OF INDONESIA AND THE VISEGRÁD COUNTRIES

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As a crucial technology for addressing global climate change and advancing carbon neutrality goals, Carbon Capture, Utilization, and Storage (CCUS) is analyzed through a comparative study focusing on Indonesia and Visegrád countries. As the first country in Southeast Asia to advance toward a commercial CCUS project in 2026, Indonesia faces several challenges in terms of economic aspects, regulatory framework, and financial feasibility. Nevertheless, it leverages its extensive practical experience in the oil and gas sector and has set an ambitious target of developing some flagship CCUS projects by 2030. In contrast, the Visegrád countries operate within the European Union's regulatory framework, which provides a more structured policy environment for CCUS deployment. Applying a socio-techno-economic approach, this study integrates the Levelized Cost of Carbon Capture (LCOCC), Social Cost of Carbon (SCC), and Levelized Cost of Electricity (LCOE) to evaluate project feasibility by calculating the Social Net Present Value (NPV Social), thereby internalizing environmental externalities. By systematically contrasting LCOCC and SCC scenarios and incorporating the Nordhaus–Stern discount rate debate, this study delineates the strategic conditions particularly the provision of subsidies through Carbon Contracts for Difference (CCFD) mechanisms and advancements in technological efficiency under which CCUS projects can achieve positive net social benefits. The findings contribute policy-relevant insights for harmonizing CCUS deployment with long-term climate mitigation objectives and broader socio-economic sustainability in both regions.

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CO_2 UTILIZATION FOR PRODUCTION OF HYDROXYBENZOIC ACIDS

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Anthropogenic carbon dioxide emissions in the last century have significantly changed the natural carbon cycle, which has caused ever-growing concern about global warming. Carbon dioxide is abundant, renewable, inexpensive, and, in the foreseeable future, environmentally harmful compound that, as such, serves as a promising feedstock in various industries. A plethora of research and review articles have been published to further motivate CO_2 mitigation and provide additional application potential [1-4].
Although most of the currently available research provides information on CO_2 reduction to formic acid/methanol/methane and the synthesis of dialkyl- or diaryl carbonates, carboxylation of reactive aromatics with CO_2 producing carboxylic acid is much less studied [1].
Nevertheless, hydroxybenzoic acids produced by action of CO_2 on phenoxides are versatile and important chemicals in the medicinal, pharmaceutical, chemical, and other industries [2-4].
In addition, the application of renewable, cheap and recyclable bases such as alkali metal hydroxides or carbonates for preparation of crucial intermediates (phenoxides) prefer this method of CO_2 utilization, being sustainable for production of long-life products such as biodegradable polyesters, etc. [2-4].
This presentation deals with the potential valorization of lignin-derived model compounds as a renewable source of aromatics and the utilization of carbon dioxide as an abundant and, in the foreseeable future, environmentally harmful compound, which results in sustainable production of value-added products of high importance in various industries such as (poly)hydroxybenzoic acids [2-4].

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GREENCHEMFORCE – CIRCULARITY IN THE CENTRAL EUROPEAN CHEMICAL SECTOR AS A PATHWAY TO CARBON NEUTRALITY

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Circularity in chemical production is essential for reducing waste, conserving finite resources, and minimizing environmental pollution, while also contributing to the broader goal of carbon neutrality. By reusing materials, closing resource loops, and increasing the use of non-fossil feedstocks, the dependence on petrochemical inputs can be reduced, leading to lower greenhouse gas emissions and more sustainable industrial processes (Keijer et al., 2019). Achieving a circular and carbon-neutral chemical industry therefore requires efficient resource management together with the development of technologies enabling the replacement of fossil resources, as well as CO_2 reduction, capture, and utilization.
Within this contribution, the project GreenChemForCE will be introduced. GreenChemForCE is a collaborative initiative promoting circular and carbon-neutral chemical practices across Central Europe by bringing together academic, industrial, and professional partners. The project focuses on three main areas: circular management of plastics, reduction and utilization of CO_2 emissions, and greener production of fine chemicals based on renewable carbon sources. Through strategic planning combined with the implementation of innovative technologies, the project aims to support a systemic transition toward a circular, low-carbon, and less fossil-dependent chemical industry.
The structure and main objectives of the project will be presented together with the outcomes of our analytical studies and the strategic approaches developed within the consortium. This overview will serve as a basis for presenting selected results from the practical part of the project, which focuses on nylon depolymerization, progress in the development of carbon capture technologies (Roth et al., 2025), and the utilization of renewable feedstocks for the synthesis of pharmaceutically relevant compounds.

UMELÁ INTELIGENCIA POMÁHA UHĽOVODÍKOVÝM TECHNOLÓGIÁM FUNGOVAŤ EFEKTÍVNEJŠIE A ČISTEJŠIE

Martin Bajus

Vďaka bezprecedentnému rozvoju umelej inteligencie vstupuje chemická technológia do radikálne novej éry. Umelá inteligencia umožňuje aplikovať vysoko-výkonné a rýchle výpočtové postupy. Metódy virtuálneho skríningu na identifikáciu chemických zlúčenín, medziproduktov a materiálov vhodných na transformáciu pre cieľové aplikácie. Využíva automatizované roboty na vykonanie nebezpečných chemických syntéz a následnú predikciu vznikajúcich produktov. Na základe údajov nazhromaždených robotickými platformami umelá inteligencia navrhuje nové experimenty. V tomto autonómnom

laboratórnom pracovnom procese zohrávajú ústrednú úlohu digitálne dátové údaje. Významne prispievajú k urýchľovaniu nových objavov v chemickej technológii.

Prechod na dekarbonizované chemické technológie so zameraním na uhľovodíkové technológie poskytujúce čistú energiou si vyžaduje kreatívne riešenia. Špičkové riešenia v chemickej technológii najčastejšie vznikajú aplikáciou moderných výpočtových a analytických metód. Vďaka tomu sa čisté petrochemikálie a palivá postupne stavajú životaschopnou náhradou fosílnych palív, napríklad vďaka elektrolytickému vodíku. Prekážky, akými sú vysoké výrobné náklady na jeho výrobu, obmedzenia efektívnosti a zložité obchodno-dodávateľské vzťahy, však bránia ich širšiemu využitiu.

Dnes je už zrejmé, že celý hodnotový reťazec čistých chemikálií a palív od výroby a skladovania až po prepravu a používanie, je možné optimalizovať pomocou umelej inteligencie. V súčasnosti už existujú niektoré pozoruhodné spôsoby, ktorými sa umelá inteligencia v chemickej technológii presadila. Sme svedkami toho, ako môže dátabankou riadená analýza, strojové učenie a hlboké strojové učenie zvýšiť efektívnosť výroby čistých petrochemikálií a palív a zároveň znížiť prevádzkové náklady a zvýšiť spoľahlivosť.

Globálny dopyt po rope a zemnom plyne porastie až do roku 2050, uviedla Medzinárodná energetická agentúra (IEA) v novembri 2025. Tým sa zásadne odklonila od svojich predchádzajúcich predikcií. Tie v minulosti predpovedali skôr plynulý prechod na čistejšie palivá. IEA dospela k tomuto prelomovému konštatovaniu práve v čase, keď energetickom sektore enormne rastie dopyt po elektrickej energii, pričom hlavným hnacím motorom jej odberu je rozvoj dátových centier a umelej inteligencie. Megatrend umelej inteligencie podporuje rast globálneho dopytu po elektrickej energii. Predpokladá sa, že americký trh s elektrinou, ktorý bol celé desaťročia oblasťou s nízkym rastom, by mal zaznamenať výrazný nárast dopytu po elektrine vďaka prieniku umelej inteligencie, a to priemerným tempom približne 20 % ročne do roku 2030.

Ropným a petrochemickým rafinériám ponúka umelá inteligencia obrovský potenciál, ako pomôcť jednotlivým procesom, aby fungovali efektívnejšie a čistejšie. Jej cieľom je predovšetkým využitie obrovského množstva už existujúcich digitálnych prevádzkových údajov. Umelá inteligencia následne cez svoje modely optimalizuje rafinérske a petrochemické procesy. Pomáha predpovedať a odhaľovať poruchy zariadení. Algoritmy AI uľahčujú integráciu obnoviteľných zdrojov energie. Umelá inteligencia má pritom neustále kontrolu aj nad prevádzkovou udržateľnosťou. Všetky spomenuté schopnosti a prednosti umelej inteligencie už dnes vstúpili do rafinérií. Viditeľne prispievajú k zlepšeniu výkonnosti spracovania ropy a zemného plynu, či už na palivá alebo chemikálie.

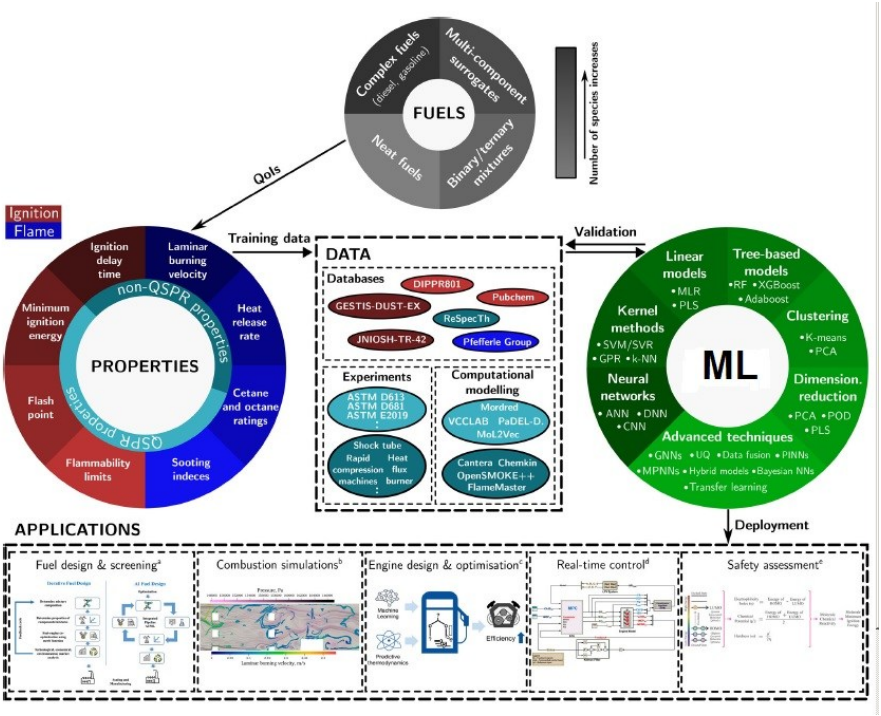
Ekonomickejšiu a škálovateľnejšiu uhľovodíkovú a vodíkovú ekonomiku umožňuje prediktívna údržba s využitím umelej inteligencie, optimalizácia elektrolýzy v reálnom čase a prepojenie inteligentných energetických sietí. Okrem toho sa ponuka a dopyt vyvažujú pomocou prognostických nástrojov riadených umelou inteligenciou, čo zaručuje čo najlepšie využitie dostupných zdrojov. V prednáške tiež demonštrujem, ako umelá inteligencia transformuje uhľovodíkové technológie a otvára dvere dekarbonizovanému energetickému ekosystému prostredníctvom prípadových štúdií a praktických aplikácií. Zaoberám sa aj aktuálnymi otázkami, akými sú potreba interdisciplinárnej spolupráce, regulačné prekážky a nedostupnosť údajov. V závere sa dotknem budúcnosti, a to

predpoveďami, v ktorých ukážem, ako inovácie riadené umelou inteligenciou urýchlia prijatie nových chemických technológií na celom svete.

Verím, že z mojej prezentácie sa dozviete viac o elementárnych princípoch a úlohách AI/ML v oblastiach, akými sú:

- Integrácia AI/ML s chemickou technológiou
- Modely AI/ML
- AI a ML v chemickom inžinierstve
- Digitálna umelá inteligencia
- Digitalizácia v rafinérskych procesoch
- CAD nástroje
- Inžiniersky diagram chemických jednotiek
- Aplikácia prompt inžinierstva v uhľovodíkových technológiách
- Najaktuálnejšie dáta pre AI a ML
- HAZOP analýza
- AI a uhľovodíkové procesy
- AI v modelovaní procesov chemickej technológie

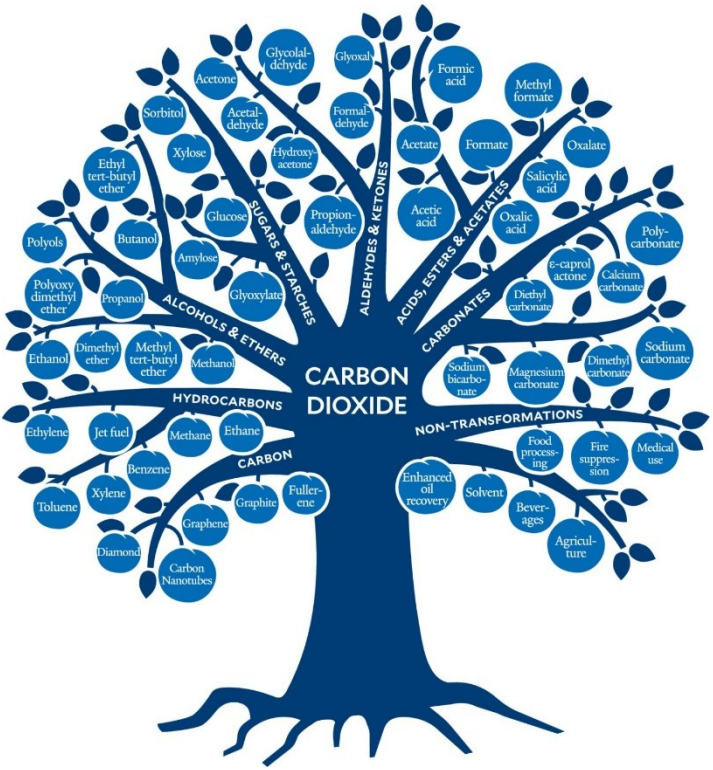
Na obrázku 1 prezentujem prehľad prednosti umelej inteligencie formou aplikácie modelov strojového učenia (ML) na predpovedanie spaľovacích vlastností palív a vlastností plameňa pri ich horení založených na kvantitatívnom vzťahu medzi chemickou štruktúrou paliva a jeho (QSPR) vlastnosťami. Pre QSPR-vlastnosti potom prezentácia poskytuje vyčerpavajúci klasifikačný rozsah predpovedí základných parametrov, akými sú: bod vzplanutia, hranice horľavosti plameňa, minimálna energia vzplanutia, teplota samovznetenia, oktánové číslo a cetánové číslo. V prípade, že kvantitatívny vzťah medzi chemickou štruktúrou paliva a jeho vlastnosťami chýba (ne-QSPR) potom sa predpovedajú nasledujúce údaje: rýchlosť laminárneho horenia, doba oneskoreného zápalu, rýchlosť uvoľňovania tepla pri horení, ale aj oktánové a cetánové číslo. Na obrázku 1 ďalej vidíme široké spektrum možností strojového učenia, ktoré sa bežne používajú v odbornej literatúre. Sú usporiadané do niekoľkých kategórií, ako: lineárne modely, stromové modely, klastrové metódy, neurónové siete, spôsoby redukcie dimenzionality, kernelové metódy a ďalšie moderné spôsoby a metódy, ktoré detailnejšie predstavím.



Obrázok 1 Sieť strojového učenia (ML) pre predikciu vlastností palív.

Popri tom obrázok 1 zahŕňa aj rôzne typy sledovaných palív, akými sú: fosílne (uhľovodíkové) palivá, alternatívne palivá: kyslíkové (alkoholy, estery, étery), palivá biologického pôvodu (biopalivá, bioplyn), e-palivá, ekologické letecké palivá (SAF), vodík a jeho deriváty (amoniak).

Spomedzi energetických materiálov, najmä na uskladnenie vodíka, zachytávanie oxidu uhličitého a metánu, si za posledné dve desaťročia značnú pozornosť získali kovovo-organické štruktúry (MOF/COF) vďaka vynikajúcim katalytickým, adsorpčným, separačným, mikroskopickým, molekulárnym a povrchovým vlastnostiam. Tieto kľúčové vlastnosti, vrátane vynikajúcich charakteristík povrchu (plocha 7000 m^2/g) , najväčšieho priemeru dutiny, limitného priemeru pórov a objemu pórov, boli základom ich štúdia. Preto sa na odhad kapacity ukladania vodíka a zachytávania oxidu uhličitého a metánu v MOF za rôznych funkčných podmienok použili výpočtové simulácie a strojové učenie, najmä konvolučná neurónová sieť (CNN) s kryštálovými grafmi (CGCNN). Integrácia simulácie Grand Canonical Monte Carlo (GCMC), strojového učenia a konvolučných neurónových sietí s kryštálovými grafmi (CGCNN) sa použila na vyhodnotenie adsorpčného a separačného účinku kovovo-organických štruktúr (MOF) a ich kompozitov s aktívnym uhlím (MOF@AC) pre radón, dusík a kyslík. Modely ML síce dosahovali vysokú prediktívnu presnosť ($R^2 > 0,9$), ale modely CGCNN boli v predpovediach rýchlejšie, aj keď o niečo menej presné.



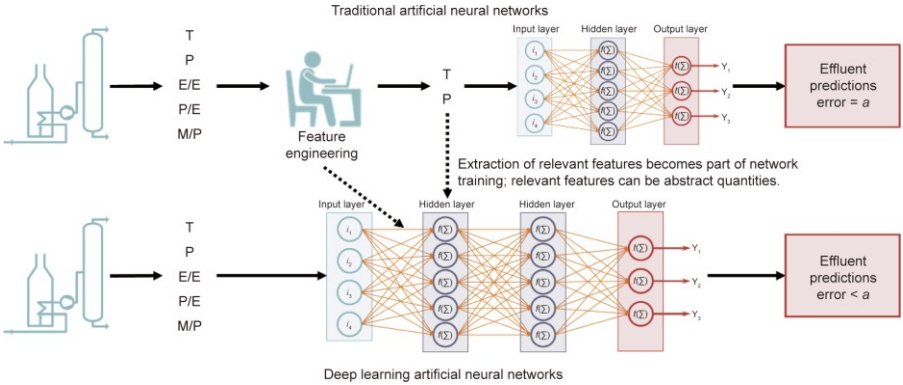
Obrázok 2 Chemický strom oxidu uhličitého prinášajúci bohatú úrodu želaného spektra chemikálií a palív od laboratórneho meradla až po priemyselnú realizáciu. (podľa technologickej vyspelosti TRL 1-9).

V prednáške využívam metaforu stromu a jej pútavú symboliku na efektívne znázornenie chemických reakcií a budúceho potenciálu využitia oxidu uhličitého. Stromy prirodzene preberajú významnú časť prirodzenej transformácie oxidu uhličitého. Chemický strom oxidu uhličitého na obrázku 2 vhodným spôsobom ilustruje širokospektrálne možnosti využívania oxidu uhličitého. Oxid uhličitý má entalpiu vzniku ($\Delta H_f°$) −393,5 kJ/mol. Z termodynamického hľadiska sa tým nachádza vo veľmi nízkom energetickom stave. Vďaka inherentnej chemickej stabilite je preto schopný dlhodobo pretrvávať v zemskej atmosfére, ako skleníkový plyn a prispievať ku globálnej zmene klímy. Cez optiku umelej inteligencie sledujem využitie oxidu uhličitého hlavne na uhľovodíkovom konári (metán) a alkoholovej vetve (metanol).

Kinetické modelovanie je základným prvkom v chemickom inžinierstve, pretože reakčné kinetické modely sú základom pre simuláciu, optimalizáciu a riadenie reaktorov. V posledných desaťročiach sa vynaložilo niekoľko výskumných snáh na získanie čoraz presnejších kinetických modelov, často založených na podrobných mechanistických údajoch.

S pokrokmi v strojovom učení sa stala novou témou výskumu možnosť aplikácie umelej inteligencie s využitím regresií založených na strojovom učení pre náhradné kinetické modelovanie. Pre účely návrhu reaktorov je hlavnou úlohou získať čo najpresnejšiu predpoveď rýchlosti reakcie pre širokú sadu parametrov. Za tým účelom je preto možné použiť prístupy založené na strojovom učení, ktoré naznačujú fyzikálne korelácie bez použitia skutočných popisov reakčných mechanizmov. Súčasná dostupnosť naznačeného (ale lacného) výpočtového postupu môže podporiť vývoj náhradných modelov riadených strojovým učením zameraných na reprodukciu kinetických korelácií v širokom rozsahu parametrov. Preto sa navrhli rôzne typy kinetických modelov. Od hlbokých neurónových sietí (DNN) v štýle čiernej skrinky až po fyzikálne podložené kinetické výrazy. Nedávno sa preukázalo, že umelé neurónové siete (ANN) dokážu efektívne predpovedať mikrokinetiku, keď sa použijú správne fyzikálne limity (skôr obmedzenia). Hlavným zmyslom takého to postupu je systematicky rozšíriť poznatky o vhodnosti metód založených na strojovom učení na odvodenie kinetických vzťahov na základe nových experimentálnych údajov získaných z komerčných katalyzátorov typu Ni/Al_2O_3 a Ni/SiO_2 vhodných pre hydrogenáciu (metanáciu) oxidu uhličitého na metán.
Pre vývoj kinetických modelov sa analyzovala široká škála dostupných regresných modelov založených na ML, vrátane modelov typu Random Forest (RF), umelých neurónových sietí (ANN) a gaussovských procesných regresií (GPR), a porovnaná so štandardným náhradným modelom PL (Power Law). Okrem toho bola najsľubnejšia regresia založená na ML porovnaná s adaptovaným modelom Langmuir-Hinshelwood-Hougen-Watson (LHHW).
Prvým typom je použitie čistého ML/DL na odhad rýchlostných konštánt alebo aktivačných energií prispôsobením databázy z experimentov, tradičného kvantitatívneho vzťahu medzi štruktúrou a reaktivitou (QSRR) a výpočtových metód (napr. MD-Molecular Dynamics; DFT-Density Functional Theory; a kMC-kinetic Monte Carlo). V poslednej dobe dochádza k rýchlemu rastu štúdií využívajúcich ML/DL na pomoc pri výpočtoch kinetických parametrov.
Komplexný súbor údajov pozostávajúci z 1547 dátových deskriptorov z 566 individuálnych experimentov v uverejnených v 84 publikáciách o katalytickej hydrogenácii oxidu uhličitého na metanol bol analyzovaný pomocou metód strojového učenia so zameraním na vývoj nových katalyzátorov. Modely typu RF vykazovali vysokú úspešnosť pri predikcii konverzie a selektivity oxidu uhličitého na metanol. Kvadratická chyba medzi predikovanými a skutočnými hodnotami (RMSE) trénovania a testovania je 2,81 (R^2 = 0,87) a 3,74 (R^2 = 0,74) pre konverziu oxidu uhličitého. Zatiaľ čo pre selektivitu na metanol bola 7,31 (R^2 = 0,94) a 12,74 (R^2 = 0,80). Podľa SHAP analýzy máme považovať reakčnú teplotu, typ nosiča katalyzátora, nanesený aktívny kov a metódu prípravy za rozhodujúce faktory ovplyvňujúce katalytickú konverziu oxidu uhličitého a selektivitu na metanol. Kým teplota ovplyvňuje konverziu pozitívne, jej vplyv na selektivitu premeny na metanol je negatívny. Analýza aktivity a reaktivity študovaných katalyzátorov (ARM) a metód ich prípravy ukázala, že použitie Ga_3Ni_5, gália, irídia, ruténia a ytria zlepšuje selektivitu premeny oxidu uhličitého na metanol, zatiaľ čo Nb_2O_5, $CuBr_2$, In_2O_3–ZrO_2 a ZnO–ZrO_2 pozitívne modifikujú nosiče katalyzátorov. Formácia katalyzátorov metódou samousporiadania indukovaného odparovaním rozpúšťadla a zrážaciou metódou zlepšuje selektivitu konverzie oxidu uhličitého na methanol. Výsledky z hodnotenia aktivity a reaktivity katalyzátorov

jednoznačne preukázali, že páry Cu–Nb_2O_5, Ga–ZnO–ZrO_2, Ru–In_2O_3 a Y–ZrO_2 sa vyznačujú vysokou selektivitou premeny oxidu uhličitého na metanol. Potvrdzujú to najmä výsledky zo štúdia posledných dvoch párov katalyzátorov, ktoré overili viacerí autori. Pri príprave heterogénnych katalyzátorov na báze medi a ruténia sú najúspešnejšie zrážacie metódy. Prípade rútenia sú veľmi prospešne aj depozičné metódy.



Obrázok 3 Porovnanie základnej neurónovej siete (ANN) s hlbokou neurónovou sieťou (DL ANN) na etylénovej pyrolýznej jednotke, T: templota; P: Tlak; E/E: Pomer etylén/etán; P/E: Pomer propylén/etán; M/P: Pomer propylén/metán; Y1: výťažok produktu 1; Y2: výťažok produktu 2; Y3: výťažok produktu 3; a: určitá (stanovená) hodnota; t(P): aktivačná funkcia.

Modelový rámec pozostávajúci zo štyroch vzájomne interagujúcich hlbokých neurónových sietí (DL ANN) predikujúcich vlastností primárneho benzínu a detailného zloženia pyrolýznych produktov sa vykreoval na základe obmedzeného počtu komerčných parametrov, alebo ľahko dostupných vlastností východiskovej suroviny a deskriptorov pyrolýzneho procesu (obrázok 3). Každá z jednotlivých sietí odovzdáva excelentný výkon, ktorý konkuruje alebo prekonáva presnosť typických online analytických zariadení a komerčne dostupných nástrojov, akým je napríklad simulačný softvér používaný v petrochemickom priemysle COILSIM1D. Použitím dvoch DL ANN sieti na reformuláciu (rekonštrukciu) detailneho zloženia východiskovej suroviny z analýzy primárneho benzínu PIONA a jej hustoty a tlaku pár sa dosiahne priemerná stredná absolutná odchylka (MAE) 0,36 % hm., ktorá zohľadňuje 28 rôznych pseudo-zložiek. Zloženie pyrolýznych produktov možno predpovedať s priemernou strednou absolutnou ochylkou 0,13 % hm., pri použití skutočného, detailného zloženia primárneho benzínu a priemernou strednou odchylkou 0,19 % hm. pri použití zloženia primárneho benzínu reformulovaného z vyššie uvedených parametrov. Docielená vysoká prediktívna presnosť v kombinácii s veľmi nízkymi výpočtovými nákladmi-vykonanie celého systému prebieha rádovo v milisekundách-robí z vyvinutých sietí veľmi vhodné siete na monitorovanie ťažko dostupných procesných parametrov v reálnom čase. Sú tiež vhodné na použitie v nových algoritmoch v reálnom

čase (RTO) s oveľa vyššou frekvenciou úprav procesu ako v súčasnosti. Pri oneskoreniach spôsobených výpočtom v ráde milisekúnd je možné uvažovať o aplikácii aj v feedforward regulácii procesov. Hoci prezentované siete boli trénované na simuláciách pre špecifickú konfiguráciu pyrolýzneho reaktora a pyrolýznej pece, začlenenie parametrov tvrdosti pyrolýzy nezávislých na reaktore medzi vstupné údaje, robí samotnú sieť nezávislou na parametroch pyrolýzneho reaktora. V dôsledku toho je prezentovaná metóda použiteľná na akýkoľvek typ reaktora bez straty výkonu. Hlavnou nevýhodou DL ANN je, že sa stráca fyzikálny a interpretovateľný význam problémov. Na detailné vyhodnotenie príčin a následkov zložitých mechanizmov, vrátnych reakčných dejov, v suvislosti s návrhovaným pyrolýznym procesom, sú stále nevyhnutné podrobné kinetické modely. Skutočnosť, že prezentované modely boli trénované na simulovaných údajoch, existuje naďalej potreba vývoja základných modelov. Avšak pre mnohé praktické aplikácie, akým je napríklad predtým spomínaná optimalizácia v reálnom čase (RTO) a riadenie procesov, sú hlavnými problémami kombinácia rýchlosti vykonávania, presnosti a jednoduchosti použitia. Vďaka flexibilite a predikčnej schopnosti DL ANN by sa v budúcnosti mohlo podobným spôsobom pristupovať aj k niekoľkým ďalším aspektom pyrolýzneho procesu uhľovodíkov, ktoré ovplyvňujú optimalizáciu pyrolýzneho zariadenia - akým je napríklad, priebeh sekundárnych reakcii a následne tvorba koksu na vnútornom povrch rúrkového pyrolýzneho reaktora.

INTESIFICATION OF CARBON DIOXIDE ABSORPTION FROM BIOGAS IN ROTATING PACKED BEDS

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Carbon capture by chemical absorption is today considered as a most mature technology to be able to capture large amounts of carbon dioxide.
Traditionally, CO_2 removal from biogas streams is carried out via absorption in stationary columns with the use of primary or secondary amines as solvents. The viability of such processes is constrained mainly by limited mass transfer. Rotating packed bed (RPB) is an apparatus for intensified mass transfer, which belongs to the high gravity (HiGee) class of process equipment. It comprises a rotor equipped with an annular packing, encased in a stationary outer shell. This approach will allow for reduction of the equipment size and operational expenses, increase the separation efficiency, and facilitate process control.
The research is carried out in three-sided cooperation between three universities in Brno, Lódž and Berlin. The research plan includes screening of solvents and development of novel rotating packings using Triply Periodic Minimal Surface structures like gyroids and diamonds that facilitate self-distribution of the liquid. Both experimental investigation and

computational simulations are used that lead to design final equipment ready for a pilot installation in a biogas station.

CARBON CIRCULARITY IN STEAM CRACKING: OPPORTUNITIES AND LIMITS OF PLASTIC WASTE PYROLYSIS OIL CO-PROCESSING

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The co-processing of plastic waste derived pyrolysis oils (PWPO) in steam cracking is widely presented as a key enabler of carbon circularity in the petrochemical industry. Yet the practical limits of integrating recycled carbon into existing large-scale cracking units remain poorly defined.
This contribution evaluates the technical, economic and regulatory feasibility of PWPO co-processing in an operating steam cracking unit under realistic industrial constraints. The assessment combines Central European market analysis, laboratory-scale Pyro-GC experiments, unit-level furnace configuration modelling and recycled content accounting.
The results confirm that currently available PWPO on the Central European market do not provide sufficiently consistent quality for direct drop-in application. Elevated chlorine and heteroatom contents exceed typical industrial tolerance limits and require upgrading or blending.
Laboratory cracking experiments indicate that PWPO co-processing increases effective feed reactivity and selectively enhances the formation of ethylene and benzene, while reducing intermediate and heavier fractions. These yield shifts were translated into an economic indicator using Cracking value. Under industrial pricing assumptions, Cracking value increases with PWPO share across all evaluated furnace configurations, although the result remains sensitive to price framework selection.
Despite favourable yield trends, furnace configuration modelling limits achievable PWPO integration to approximately 9-14 % of total unit feed. Within this technically achievable range, recycled content targets are generally not fulfilled. Only under the least restrictive allocation methodology can a 30 % recycled content target (2030 target) in polymer intermediates be achieved.
The results demonstrate that the limiting factors of PWPO integration are not primarily cracking chemistry, but feedstock quality, furnace allocation and regulatory accounting rules. The study highlights the gap between recycled content ambitions and the operational constraints of existing steam cracking infrastructure.

INFLUENCE OF ALTERNATIVE FEEDSTOCK COMPOSITION ON CARBONACEOUS DEPOSIT FORMATION DURING HYDROCARBON PYROLYSIS

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Increasing demands for sustainability and feedstock diversification in the petrochemical industry are driving interest in alternative hydrocarbon feedstocks, such as pyrolysis oils derived from waste plastics. However, these unconventional feeds can significantly affect reaction kinetics and the mechanisms of carbonaceous deposit formation during steam cracking. Enhanced coke formation leads to reduced heat-transfer efficiency, increased energy consumption, and more frequent decoking shutdowns, all of which negatively impact the economics and reliability of ethylene production units.
This work aims to systematically evaluate how the composition of selected alternative feedstocks influences the rate, mechanism, and morphology of carbonaceous deposits formed during high-temperature pyrolysis. The study integrates detailed feed characterization (SimDist, PIONA/SARA analysis, ICP-OES) with micro-pyrolysis experiments (Pyro-GC) and semi-industrial testing using a dedicated coking unit (Pylot). The resulting deposits are examined using SEM-EDX to determine their structure and elemental composition.
The collected data enable prediction of coking tendencies during co-pyrolysis of conventional and alternative feedstocks, estimation of cycle-length impacts, and formulation of guidelines for optimizing feedstock blending strategies. The results contribute to a deeper understanding of coke formation mechanisms and support the safe, efficient, and economically viable integration of alternative feedstocks into modern petrochemical processes.

POWER-TO-LIQUID TECHNOLOGIES OVERVIEW

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Power-to-Liquid (PtL) technologies represent a rapidly advancing pathway for producing renewable, electricity-based synthetic fuels that support deep decarbonization of hard-to-electrify sectors such as long-haul aviation, maritime transport, and heavy-duty road transport. A fundamental challenge for CO_2 utilization lies in the high thermodynamic stability and low reactivity of the CO_2 molecule, requiring significant external energy input, optimized reaction conditions, and highly active catalysts.
Electrofuels (e-fuels) based on green hydrogen and captured CO_2 enable a closed carbon cycle while leveraging abundant primary resources such as water and air. Among these,

e-hydrocarbons offer excellent scalability and compatibility with existing fuel infrastructure, though their production remains energy-intensive due to hydrogen generation and CO_2 conversion steps.

E-diesel is an important candidate for decarbonizing heavy-duty transport and maritime applications. Produced via water electrolysis, reverse water–gas shift (RWGS), and Fischer–Tropsch synthesis (FTS), e-diesel is fully compatible with current engines and distribution systems. Its drop-in nature allows immediate adoption without significant infrastructure upgrades.

Synthetic aviation fuels (e-SAF) derived from renewable hydrogen and captured CO_2 offer one of the most promising options for reducing greenhouse gas emissions. FTS-based e-kerosene, containing C8–C16 hydrocarbons, meets stringent performance and safety requirements and can be blended with fossil jet fuel according to ASTM D1655. Its low aromatic and sulfur content enables cleaner combustion. However, challenges remain regarding the energy intensity of green hydrogen production and the availability of low-carbon CO_2.

Alternative pathways, such as Methanol-to-Jet (MTJ) and Ethanol-to-Jet (ETJ), convert renewable methanol or ethanol to olefins, followed by oligomerization, hydrogenation, and fractionation to yield synthetic paraffinic kerosene (SPK) compliant with ASTM D7566. MTJ technologies offer promising efficiency gains and operate at lower pressures and temperatures compared with FTS.

Methanol synthesis from CO_2 and hydrogen remains complex but enable performance comparable to conventional CO-based routes.

Overall, **PtL and e-fuel technologies** present scalable, infrastructure-compatible solutions for achieving deep reductions in lifecycle emissions. Their widespread deployment will depend on advances in electrolyzer technology, CO2 capture efficiency, catalyst development, and the availability of large amounts of low-cost renewable electricity.

Other-wise this is dead-end.

DIGITAL AND GREEN TRANSFORMATION OF THE PLASTICS INDUSTRY

LECTURES

DOPADY DIGITÁLNÍ A ZELENÉ TRANSFORMACE NA PLASTIKÁŘSKÝ PRŮMYSL ČR

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V rámci prezentace budou představeny klíčové výstupy z aktualizovaných strategických dokumentů České technologické platformy Plasty (ČTP Plasty), které reflektují aktuální výzvy a příležitosti plastikářského průmyslu v České republice v kontextu evropských cílů udržitelnosti a digitalizace. ČTP Plasty, existující již 16 let s 28 členy a zkušenostmi z mnoha domácích ale i mezinárodních projektů, se dlouhodobě zaměřuje na podporu výzkumu, vývoje a inovací v oblasti plastů, a tedy i na aktuální témata průmyslové transformace.
Klíčová témata jsou obsažena ve Strategické výzkumná agendě (SVA), která definuje dlouhodobé priority výzkumu, jako jsou pokročilé polymerní materiály, recyklace a bio-based alternativy. Aktualizace SVA vychází z analýzy budoucích trendů a slouží jako základ pro směřování inovačních aktivit.
Doplňujícím materiálem je pak aktualizovaný Technologický foresight, který mapuje možné scénáře vývoje plastikářského průmyslu do roku 2030 a dále. Dokument identifikuje klíčové trendy, jako je přechod na cirkulární ekonomiku, regulace emisí, využití umělé inteligence a konkurence z Asie, a navrhuje strategie pro adaptaci českého průmyslu.
Nejnovějším příspěvkem podpory plastikářského sektoru je pak Akční plán digitální a zelené transformace, vzniklý v rámci projektu Plasty V podporovaného OP TAK. Tento plán přináší návrh konkrétních opatření pro zelenou transformaci (recyklace, snížení uhlíkové stopy, udržitelné suroviny) i digitální (automatizace, Průmysl 4.0, AI ve výrobě), včetně časového harmonogramu a odpovědností za jejich implementaci do praxe.
Dokumenty jsou vzájemně propojené, technický foresight popisuje očekávané scénáře budoucího vývoje, SVA priority a akční plán konkrétní kroky. Společně pak dokumenty podporují konkurenceschopnost českého plastikářství v souladu s aktuální politikou EU.
Plné texty zmíněných dokumentů lze nalézt na www.tp-plasty.cz v sekci dokumenty.

METHODOLOGICAL CHALLENGES IN LCA OF PLASTIC RECYCLING

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Life Cycle Assessment (LCA) is a powerful tool for quantifying environmental performance of recycling technologies, yet its outcomes are heavily influenced by methodological choices. This presentation examines how economic allocation of coproducts, substitution modelling of recyclate quality and baseline scenario selection act as key levers shaping LCA results and subsequent investment and regulatory decisions in plastic recycling.

Using marked plastic waste separation systems as case study, the presentation demonstrates these effects through three concrete methodological examples. First, economic allocation of separated waste streams assigns a disproportionate share of

upstream impacts to high-value fractions like single origin plastics based on market prices. Second, guaranteed material composition from marking enables full virgin substitution credits, unlike non-guaranteed recyclate requiring reduced substitution factors due to compromised material properties. Third, selecting appropriate baseline scenarios for waste management—such as sorting followed by chemical recycling versus incineration or material recovery for pallets—is crucial, as different reference pathways lead to fundamentally different conclusions.

These examples illustrate why LCA sensitivity to methodological choices requires transparent reporting for meaningful environmental benchmarking. The presentation discusses current European debates on standardisation and provides guidance for critically evaluating LCA studies in waste management and circular economy.

CARBON NANOMATERIALS FROM METHANE PYROLYSIS AS FUNCTIONAL ADDITIVES FOR ADVANCED POLYMER COMPOSITES

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Methane pyrolysis is a promising pathway for the sustainable production of hydrogen and carbon nanomaterials without direct CO_2 emissions. In this process, methane decomposes into molecular hydrogen and solid carbon according to the reaction $CH_4 \rightarrow C + 2H_2$. While hydrogen is widely discussed as a clean energy carrier, the simultaneous formation of carbon nanostructures creates new opportunities for advanced material applications.
In this work, carbon nanoparticles produced via methane pyrolysis were investigated as functional additives for polymer composite systems. Particular attention was paid to the morphology, size and surface properties. The nanostructures were characterized using scanning electron microscopy, Raman spectroscopy and surface area analysis to determine their structural and physicochemical properties.
The incorporation of these carbon nanomaterials into polymer matrices offers several advantages, including improved electrical conductivity, enhanced mechanical strength and increased thermal stability. Such materials may find applications in conductive polymer composites, electromagnetic interference shielding, sensors, advanced air filtration systems and energy technologies.
The proposed approach links hydrogen production with advanced materials manufacturing. By valorizing the solid carbon fraction generated during methane pyrolysis, the overall process economics and sustainability can be improved. Carbon

nanostructures with tailored surface properties serve as functional components in next-generation air filtration materials.
The financial support of the TACR NCC MATCA II subproject “Integrated Microwave Plasma Technology for the Production of Hydrogen and Carbon Nanostructures for Intelligent Filtration Systems (PLAZTECH)” No. TN02000069/022 and the program “Strategy AV21” of the Czech Academy of Sciences, specifically work package VP27 Sustainable Energy (Renewable energy resources and distributed energy systems), are gratefully acknowledged.

FABRICATION OF BIOPOLYMER IN COOPERATION OF SILVER NANOPARTICLES ACT AS A SUSTAINABLE ALTERNATIVES TO REPLACE SINGLE-USE-PLASTICS

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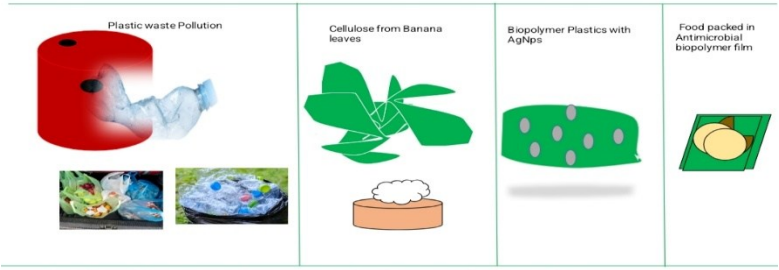

The widespread application of Single-Use-Plastics has created serious environmental challenges due to their non-biodegradable nature and accumulation in our ecosystem. In this research, biodegradable biopolymer films were prepared as a sustainable alternative to Single-Use-Plastics. Natural polymer matrices were synthesized and combined with the silver nanoparticles (AgNPs) to increase their functional properties. The addition of AgNPs improved the mechanical strength, stability, and antimicrobial activity of the biopolymer films. The developed films were characterized using various analytical techniques such as XRD, FTIR, UV, UV visible-NIR, DLS, SEM and Tensile test were performed to evaluate their structural, functional and mechanical properties. The results indicated that in cooperation of silver nanoparticles significantly enhanced the performance of the biopolymer matrix as compared with the non-addition of silver nanoparticles in the biopolymer material. The developed biopolymer–AgNP composite showed promising potential as an eco-friendly material for food packaging and other sustainable applications, offering an efficient route to decrease the dependence on Single-Use-Plastics and mitigate environmental pollution way towards the Circular Economy concept.

INORGANIC TECHNOLOGY

LECTURES

PERFORMANCE AND DEGRADATION MECHANISMS OF MONIFEP MODIFIED CARBON FIBRES UNDER HYDROGEN EVOLUTION CONDITIONS IN ACIDIC AND ALKALINE ENVIRONMENT

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Hydrogen is considered a promising alternative to fossil fuels due to its potential as a clean energy carrier. It can be produced from water by electrolysis powered by renewable energy sources. However, the sluggish kinetics of the hydrogen evolution reaction (HER) in alkaline media and the reliance on platinum-based catalysts in acidic media limit the large-scale application of water electrolysis. Therefore, the development of stable, low-cost electrocatalysts with high activity and durability remains highly desirable.
Non-precious metal catalysts based on Mn, Fe, Co, or Ni have been widely investigated in forms such as oxides, (oxy)hydroxides, phosphides, nitrides, and selenides. Among them, bi- and trimetallic transition-metal phosphides exhibit near-platinum-like HER activity and potential for operation in both acidic and alkaline media. Their performance arises from the synergistic interaction between metal and phosphorus species. The incorporation of phosphorus forms ionic $Ni^{\delta+}$-$P^{\delta-}$ bonds, where P sites promote hydrogen adsorption in acidic media, while, in alkaline media, phosphorus weakens the O–H bond and facilitates water dissociation. Nevertheless, phosphides are often synthesized as powders that must be deposited onto electrodes, increasing interfacial resistance and potentially decreasing activity.
Here, flexible, free-standing fibrous C/MoNiFeP electrodes were prepared by electrospinning and tested in 0.5 M H_2SO_4 and 1 M KOH using a standard three-electrode configuration. The electrodes exhibited good activity in acidic (η_{10} = –344 mV) and alkaline media (η_{10} = –223 mV). Stability tests revealed significant surface reconstruction in acidic conditions, whereas stable performance was maintained in alkaline media during prolonged operation.

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EFFECT OF PYROLYSIS TEMPERATURE ON HYDROGEN-EVOLUTION REACTION CAPABILITIES OF HIGH-ENTROPY CARBIDES

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High-entropy materials are typically formed from four or more elements with similar atomic sizes to promote stable single-phase solid solutions, resulting in unique physico-chemical characteristics compared to their individual components. High-entropy carbides (HEC), composed of two interpenetrating sublattices of transition metals and carbon, exhibit exceptional hardness and electrical conductivity. Their broad distribution of hydrogen adsorption energies creates a catalytical “sweet spot” that statistically satisfies the Sabatier principle, making HEC promising catalysts for the hydrogen-evolution reaction (HER).
Composite ceramic nanofibers based on TiZrHfNbTaC HEC were prepared from identical electrospun precursor fibers. Nb, Ta, and Hf chlorides were used as ceramic precursors together with titanium isopropoxide and zirconium propoxide, while polyacrylonitrile served as the carrier polymer. The as-spun fibers were pyrolyzed at 1100–2100 °C, yielding porous, flexible ceramic fibers. Phase and chemical composition were verified by XRD and SEM/EDS. Samples were also tested for HER activity. Measurements were performed in alkaline and acidic water electrolysis using a three-electrode setup. Samples were additionally evaluated for stability and their their electrical conductivity was also determined.
Increasing temperature promoted progressive carbothermal reduction and crystallization of HEC. Lower-temperature XRD patterns showed broad reflections and residual HfO_2, indicating incomplete conversion. At ≥1900 °C, sharp carbide peaks dominated and oxide phases disappeared. Higher temperatures also transformed the amorphous carbon matrix into a highly ordered graphitic structure with aligned crystalline domains, enhancing carbon-layer ordering. This led to enhancement of HER activity in both alkaline and acidic media.

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CARBON NANOTUBES IN NEW ELECTROCATALYTIC SYSTEMS FOR ELECTROLYTIC HYDROGEN PRODUCTION

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Hydrogen production through water electrolysis is one of the key technologies for the development of sustainable energy systems. The project aims to develop and study nickel-based nanocomposite coatings using carbon nanotubes (CNT) as electrocatalysts applicable in water electrolysis. CNT coatings have a variety of advanced properties especially their high electrical conductivity, large specific surface area, and excellent chemical stability.
The experimental part is focused on the preparation, modification and characterisation of CNTs nanocomposite coating deposited on nickel foam by electrodeposition. First, with a constant concentration of CNT to the Ni-Fe electrolyte, it was studied different additions of surfactants in the electrolyte. The aim was identification of the differencies in microstructure and adhesion of CNTs nanocomposite coating to Ni foam. Lastly, the catalytic activity of the prepared materials was studied. It was found that CNT coating represent a promising catalyst for hydrogen evolution reaction in alkaline water electrolysis.
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ENHANCING PT UTILIZATION VIA IN-PLANE AND THROUGH-PLANE GRADIENTS IN PEMFC CATHODES

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Proton exchange membrane fuel cells (PEMFCs) offer efficient, sustainable power generation, but their widespread commercialization is, beside others, heavily constrained by the high cost of Pt catalysts. To optimize Pt utilization and mitigate degradation resulting from the inherent non-uniform distributions of reactants and potentials during operation, manufacturing functionally graded cathode catalyst layers (CLs) has emerged as a promising strategy. This approach involves the deliberate spatial variation of CL properties such as Pt loading and structural porosity to match the electrode structure to the specific local operating requirements.
A steady-state, isothermal, two-phase numerical model was employed to evaluate these architectures. The model utilizes a spherical agglomerate framework to accurately resolve

species transport, multi-phase water dynamics, charge conservation, and reaction kinetics. In-plane (IP) and through-plane (TP) gradients were simulated while maintaining a constant average cathode loading. The model was validated against experimental polarization curves from inkjet-printed CLs.
Results demonstrate that IP gradients concentrating Pt towards the gas flow outlet successfully mitigate local oxygen starvation. This outlet-biased approach consistently yields higher currents and homogenizes local reaction rates across both activation/ohmic controlled (0.6 V) and mass-transport-limited (0.3 V) regimes. For TP gradients, adjusting structural porosity exerted a dominant effect over pure Pt relocation. Expanding porosity towards the gas diffusion layer facilitated oxygen diffusion, substantially lowering mass transport losses at high loads. Conversely, enriching Pt near the membrane minimized protonic transport resistance, significantly enhancing high-voltage efficiency.
Ultimately, combining an outlet-biased IP gradient with a membrane-biased TP Pt distribution maximized synergistic performance. By linking advanced multi-physics modeling with practically realizable structural designs, this work establishes robust guidelines for engineering high-performance, low Pt loaded PEMFCs.

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IDENTIFICATION OF POTENTIALLY HAZARDOUS OPERATING REGIMES IN AMMONIA SYNTHESIS BASED ON DYNAMIC MODELLING

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This work focuses on ammonia as one of the key products of the global chemical industry. The nonlinear nature of the ammonia synthesis process is investigated, with particular emphasis on the analysis of its dynamic response to variations in one or more operating parameters. Ammonia synthesis belongs to the class of highly exothermic reactions, which may become potentially hazardous under abnormal operating conditions. Within the scope of the research, sensitivity analysis is performed under both steady – state and dynamic conditions, enabling the assessment of process stability and the identification of parameter regions in which unpredictable or unstable operating regimes may occur. A systematic identification of hazardous operating states is carried out using the HAZOP philosophy, adapted for the analysis of numerical simulation results. The response of the ammonia synthesis loop to deviations in various process parameters within defined ranges is examined. The steady – state simulation of the entire process is developed using the Aspen Plus software. A dynamic model of the ammonia synthesis loop is implemented in

the Aspen Plus Dynamics environment, allowing for the analysis of the temporal evolution of the process under various disturbance scenarios. The results of this work demonstrate that dynamic modelling combined with sensitivity analysis represents an effective tool for improving industrial safety and understanding the behavior of complex ammonia synthesis systems.

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WHEN ADSORPTION IS TOO FAST: PCBS ON COMMERCIAL ACTIVATED CARBONS

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Introduction

Polychlorinated biphenyls (PCBs) are persistent organic pollutants characterized by high chemical stability, hydrophobicity, and resistance to natural degradation processes. Due to their historical industrial use as dielectric fluids and plasticizers, PCBs remain widespread in aquatic environments, where they pose long-term ecological and human health risks. Although adsorption using carbon-based sorbents is widely applied for PCB removal, the performance differences among commercially available sorbents and the mechanisms governing ultra-fast uptake under low-concentration conditions remain insufficiently understood.

Methodology

Three commercially sourced activated carbon sorbents, including both legacy and currently available products, were evaluated for PCB removal from aqueous solutions containing technical mixtures (Delor 103 and Delor 106). Sorbents were characterized by BET surface area analysis, SEM imaging, surface charge measurements, and surface chemical analysis. Batch adsorption experiments were conducted at low PCB concentrations and short contact times (1-20) min. PCB concentrations before and after treatment were quantified by GC-ECD following liquid–liquid extraction.

Results

All investigated sorbents exhibited very rapid PCB uptake, achieving near-complete removal within minutes. Congener-specific differences were observed during the initial stages of adsorption, particularly for higher-chlorinated PCBs. Despite notable differences in textural and surface chemical properties among the sorbents, their overall removal efficiencies were similarly high under ultra-fast adsorption conditions. Conventional kinetic models showed limited mechanistic interpretability due to the rapid approach to equilibrium.

Conclusion

Commercial activated carbon sorbents provide highly efficient and rapid removal of PCBs from aqueous solutions under low-concentration conditions. Under ultra-fast adsorption regimes, operational performance metrics such as time-to-removal and dose efficiency are

more informative than classical kinetic parameters. These findings support the practical use of commercial carbon sorbents for rapid PCB decontamination and highlight limitations of conventional kinetic modelling for high-affinity adsorption systems.

Acknowledgment
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ELECTROCHEMICAL REMEDIATION OF POLYCHLORINATED BIPHENYLS: STATE OF THE ART, GAPS, AND ENGINEERING PATHWAYS FORWARD

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Introduction
Polychlorinated biphenyls (PCBs) are persistent organic pollutants characterized by high chemical stability, hydrophobicity, and resistance to conventional remediation technologies. Despite more than four decades of research on electrochemical PCB degradation, practical implementation remains limited, and the field has not matured at the same pace as other electrochemical remediation or energy-related subfields.

Methodology
A critical literature analysis was conducted covering approximately 31 published studies on electrochemical PCB remediation, encompassing direct electrochemical reduction, indirect oxidation (Electro-Fenton and photo-assisted systems), mediated electrochemical oxidation, and hybrid approaches. The reviewed studies were systematically compared in terms of degradation mechanisms, electrode materials, electrolyte environments and other factors, energy consumption, mineralization indicators (TOC removal and CO_2 yield), and by-product formation. Engineering and scale-up considerations were evaluated through reported reactor configurations and transport limitations.

Results
The literature reveals that most studies report PCB removal rather than true mineralization, with limited quantitative data on TOC removal or CO_2 yields. Performance metrics and energy consumption are inconsistently reported, preventing meaningful comparison between electrochemical pathways. Reactor-scale challenges including mass-transfer limitations, non-uniform current distribution in porous electrodes, electrode fouling, and secondary reactions, remain largely unaddressed. Compared with more mature electrochemical subfields, electrochemical PCB remediation shows limited integration of mechanistic electrochemistry, standardized benchmarking, and reactor-level modeling.

Conclusion
Electrochemical remediation of PCBs remains scientifically promising but technologically immature. Progress toward scalable implementation requires coupling fundamental electrochemical analysis with reactor engineering, energy efficiency metrics, and

standardized performance reporting. This work outlines a framework for advancing electrochemical PCB remediation from lab-scale studies toward practical and sustainable environmental applications.

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THERMAL BEHAVIOR AND OPTICAL PROPERTIES OF RARE-EARTH-ELEMENT–DOPED ALUMINATE GLASSES

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Alumina-rich glasses exhibit superior optical, thermal, and mechanical performance. Within the $Al_2O_3 – RE_2O_3$ compositional domain, glasses with garnet-type stoichiometries constitute particularly promising host matrices, in which dopant incorporation can effectively induce modifications that enhance functional properties. Yb^{3+}/Er^{3+} co-doped aluminate glasses represent attractive precursor materials for the fabrication of phosphors with favorable photoluminescence characteristics, which have the potential to replace commercially used counterparts. Conventional production routes, however, typically rely on capital- and energy-intensive equipment and are associated with limited throughput. A more resource-efficient and scalable strategy can be developed by combining the synthesis of glass microspheres via flame synthesis (FS) with subsequent hot-press (HP) sintering. A detailed understanding of the crystallization mechanisms and associated kinetics is essential for defining appropriate HP processing conditions, either to suppress undesirable crystallization or to selectively promote and control it to obtain the targeted glass-ceramic microstructure.

In this study, optical properties and thermal behavior of optically active glasses with garnet-type compositions in the $Al_2O_3 – Yb_2O_3 –Y_2O_3 – Er_2O_3$ and $Al_2O_3 – Yb_2O_3 – Er_2O_3$ systems were investigated. The samples were synthesized by combining the Pechini sol–gel method with flame synthesis. Thermal behavior was characterized by differential scanning calorimetry (DSC), complemented by scanning electron microscopy (SEM) and X-ray powder diffraction (XRD). The thermal behavior was examined in the temperature range 30 – 1100 °C. Glass transition was observed at approximately 864 °C, followed by crystallization at temperatures exceeding 900 °C. Subsequently, the crystallization behavior was investigated by a series of non-isothermal DSC measurements at different heating rates, supported by crystallization experiments under isothermal conditions at the

temperatures corresponding to the maxima of the crystallization peaks. Kinetic triplets were determined using the Johnson–Mehl–Avrami–Kolmogorov (JMAK) model. The combined SEM, XRD, and kinetic analyses indicated a chemically controlled crystallization mechanism, with a nucleation rate linearly dependent on time and either 2-D (for ≥5.0 mol.% Er_2O_3) or 3-D (in the presence of Y_2O_3 and/or ≤3.0 mol.% Er_2O_3) growth of a cubic garnet phase. The thermal stability and glass-forming ability of the investigated systems were significantly influenced and generally improved by increasing Er_2O_3 content. Optical characterization confirmed these materials as promising candidates for green and red phosphors when excited by ultraviolet and infrared radiation, respectively.

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INORGANIC TECHNOLOGY

POSTERS

PREPARATION OF EARLY TRANSITION METAL IONS WITH LOW VALENCY AND OPEN COORDINATION SPHERE FOR CATALYTIC APPLICATION V(II)–FERRIERITE STUDY

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Divalent cations stabilized in the framework of silicon rich zeolites represents redox catalytic sites applied in number of redox catalytic reactions (e.g. N_2O and NOx abatement, selective oxidation of methane to methanol). Nevertheless, the attention was focused on metals with significantly preferred divalency as Cu, Co, Ni, Fe. In this paper, we present the first report on the preparation of silicon rich zeolite (of ferrierite topology with Si/Al 8.5) with bare divalent vanadium cations in extra-framework cationic sites. Moreover, activity of pairs of cooperating V(II) ions in binuclear cationic sites towards small important molecules is discussed.

CHEMICAL DISPOSAL OF SALT SLAG FROM ALUMINUM RECYCLING

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Hliník představuje klíčovou surovinu pro moderní průmysl, přičemž jeho význam v EU podtrhuje nedávné zařazení na seznam kritických surovin (CRMA). Vzhledem k vysoké energetické náročnosti primární výroby nabývá na významu sekundární produkce hliníku. Ta je však spojena se vznikem solné strusky, která je pro svou reaktivitu a složení klasifikována jako nebezpečný odpad. Předložená práce se zabývá procesy chemické separace složek strusky s cílem minimalizovat environmentální rizika a zajistit opětovné využití surovin v rámci cirkulární ekonomiky. Složení solné strusky je velice proměnlivé a skládá se ze zbytků tavicích solí (NaCl, KCl), oxidů hliníku, kovového hliníku a nekovových složek (nitridy, karbidy, sulfidy, fosfidy). Hlavní metodou chemického zpracování je hydrometalurgické zpracování (loužení např. vodou), případně kombinované s mechanickým předzpracováním. Problematickou částí celého procesu je hydrolýza nekovových složek, při níž se uvolňují plyny (amoniak, metan, sulfan, fosfan), které musí být zachyceny a čištěny. Při hydrometalurgickém zpracování solné strusky, při dodržení optimálních podmínek, lze z procesu získat tavidla (KCl, NaCl), která lze znovu použít. Práce zároveň vyhodnocuje kinetiku uvolňování plynných produktů hydrolýzy a navrhuje efektivní způsoby jejich neutralizace. Výsledkem chemického zpracování je uzavřený procesní cyklus, který eliminuje nutnost skládkování, snižuje náklady na nákup nových tavidel a produkuje inertní materiály využitelné ve stavebnictví nebo při výrobě žáruvzdorných materiálů. Alternativou je vysokoteplotní zpracování spočívající v zahřátí

strusky na vysokou teplotu (cca 1600 °C), což vede k odpaření solí, které jsou následně zachyceny. Tento proces je velice energeticky náročný, ale eliminuje nutnost vodního hospodářství.

Literatura:
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LINKING VISCOSITY AND DIFFUSION WITH CRYSTAL GROWTH KINETICS IN $GE_{25}S_{75}$ BULK GLASS

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Chalcogenide glasses have long attracted considerable interest, owing to their unique optical and electrical properties. They exhibit high IR transmittance and a relatively high refractive index, making them suitable for infrared optics and the fabrication of optical fibers. Furthermore, the change of optical properties accompanying the amorphous-crystalline phase transition enables their use in data storage, optical switches, photonics components, and energy storage devices. A comprehensive understanding of kinetics and physical properties is essential for optimization and technological application of these materials.

For crystals to grow, structural units need enough mobility. Higher mobility can be observed at higher temperatures, especially in the undercooled melt region, which is a temperature range above the glass transition temperature. To fully understand the kinetic properties of $Ge_{25}S_{75}$ material, a series of crystallization and viscosity experiments were performed.

The viscosity properties of amorphous bulk samples were studied using the thermomechanical analysis (TMA), and the obtained viscosity data were then described by the MYEGA viscosity model. The crystallization was initiated by annealing amorphous samples at high temperatures (640-780 K), with the crystals observed using the IR microscopy, enabling direct observation of the growing spherulitic β-GeS_2 modification. The dependency of the crystal growth rate (calculated as a change in the crystal's length over time) on temperature was described using a normal growth model. This model extrapolates data over a broad range of temperatures. From its parameters, a direct calculation of the coefficient of self-diffusion provides valuable insight into the transport mechanisms in chalcogenide glasses.

Acknowledgments
This study was supported by the Czech Science Foundation under grant no. 24-10480S, by the Internal Grant Agency of the University of Pardubice under grant number SGS_2026_006 and by the Selected Research Teams program of the University of Pardubice.

ENVIRONMENTAL PROTECTION TECHNOLOGY

LECTURES

HEAR TRANSFER FLUID RECYCLING, PRACTICAL EXPERIENCE

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Antifreeze fluids typically contain water, glycol, corrosion inhibitors, and various additives (dyes, antifoaming agents, etc.). After several years of operation, corrosion products and degradation products accumulate in the fluid. The main goal of recycling is to remove these contaminants and additives, because aged additives may be incompatible with newly formulated additive packages. The conventional approach relies on distillation to remove water, additives, and degradation products. In contrast, we selected electrodialysis as the core recycling technology. This method offers advantages such as low energy consumption and minimal heat generation, although it also has limitations: it cannot remove water from glycol, and it is not cost-effective for heavily contaminated antifreezes. The waste antifreeze first undergoes coarse filtration. After sedimentation, coagulants and activated carbon are added to remove organic and inorganic impurities, dyes, and oil residues. Subsequent fine filtration removes the coagulants and activated carbon. Electrodialysis is then used to reduce the content of inorganic and organic salts, yielding an aqueous glycol solution with an overall process efficiency of 90 %. As a manufacturer of antifreeze fluids, we reuse the recovered glycol in our own production. The recyclate is concentrated to the required glycol content and supplemented with new additives. The resulting coolant meets the same performance requirements as coolant produced from virgin raw materials.

ADVANCED METHODS FOR BIOGAS PURIFICATION

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Reducing the CO_2 and H_2S content in biogas is one of the major challenges currently faced by the biogas industry. In the Czech Republic, financial support for biogas plants is gradually decreasing, making the operation of small and medium-sized plants increasingly unsustainable. One possible solution is upgrading biogas to biomethane, which, due to its higher CH_4 content, enables more efficient transportation and storage. Membrane separation is a promising approach because of its relatively low energy demand and modular design.
This work focuses on water-swollen thin-film polymer membranes, which are commercially available even in the form of membrane modules and therefore represent a cost-effective option for CO_2 separation. These membranes are currently being tested mainly for CO_2 removal from biogas, with the aim of achieving sufficiently high selectivity of CO_2 over major gas components such as CH_4 and N_2. For economically feasible

operation, a CO_2 selectivity of at least 10 is generally considered necessary. In addition to CO_2 separation, this work also addresses H_2S removal from biogas using an inexpensive selective sorbent capable of regeneration when exposed to oxygen and water vapour.
Experimental measurements were carried out both in a permeation cell used for membrane characterization and in a membrane module originally designed for reverse osmosis. In the module experiments, separation of CO_2 from a model CO_2/CH_4 gas mixture was studied, with the aim of obtaining highly concentrated methane in the retentate stream. H_2S removal was investigated using a simple experimental setup, and the obtained data were used to determine sorbent capacity and regeneration efficiency. The results provide a basis for further optimization of operating conditions and for the design of multistage systems for biogas upgrading.
Acknowledgement:
This work is supported within the project „Waste as an alternative source of energy“, reg. nr. CZ.02.01.01/00/23_021/0008590 under the Programme Johannes Amos Comenius.

STANOVENÍ LÁTEK S ORGANICKY VÁZANÝM FLUOREM VE VZORCÍCH VOD DLE NORMY ISO 18027

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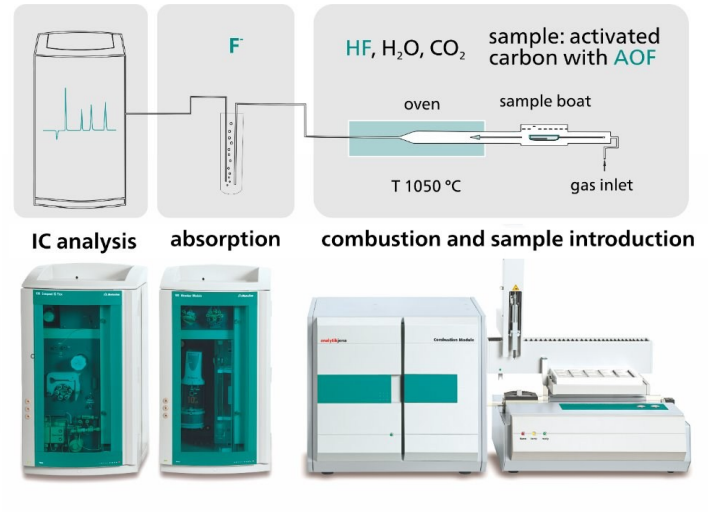
PFAS (per- a polyfluorované alkylové látky) představují skupinu téměř 10 000 organofluorovaných sloučenin. Tyto člověkem vytvořené látky, často označované jako „věčné chemikálie“, jsou vysoce perzistentní a některé z nich mají tendenci se hromadit a zadržovat v životním prostředí. Z tohoto důvodu je stále více těchto sloučenin klasifikováno jako toxické, protože představují riziko pro lidské zdraví i životní prostředí.
Tyto negativní dopady na zdraví přiměly vládní a normalizační orgány k přijetí opatření proti nejškodlivějším PFAS. To vedlo k požadavkům na vývoj vhodných analytických metod pro sledování a regulaci těchto látek. Cílená analýza PFAS je složitá a vyžaduje nákladné přístrojové vybavení a neposkytuje celistvý obraz látek s organicky vázaným fluorem, které se zadržují v životním prostředí. Naproti tomu stanovení necílených souhrnných parametrů ve fromě adsorbovatelného organického fluoru (AOF) představuje jednodušší a dostatečný způsob screeningu přítomnosti PFAS. Analýza AOF pomocí spalovací iontové chromatografie (CIC) je uznávanou screeningovou metodou pro stanovení PFAS ve vzorcích vody. Norma ISO 18027 popisuje použití kombinace pyrohydrolytické oxidace a iontové chromatografie (CIC, Obr. 1) nejen pro analýzu AOF ale také AOCl, AOBr a AOI ve vzorcích vod— pro kterou společnost Metrohm vyvinula robustní a spolehlivé řešení.



Obr. 1 princip spalovací iontové chromatografie

APPLICATION OF ELECTRODIALYSIS FOR *N,N*-DIBUTYLIMIDAZOLIUM CHLORIDE RECOVERY FROM WASTEWATER – EFFICIENCY, MEMBRANES CHARACTERISTICS AND CHEMICAL STABILITY OF THE RECOVERED IONIC LIQUID

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Ionic liquids (ILs) are liquid molten salts. Due to their low vapour pressure, non-volatility and non-flammability, they are often referred to as the „solvents of the future". An example of an IL is *N,N*-dibutylimidazolium chloride ([BBIM]Cl). However, due to its high price and toxicity, it is important to recover it from wastewater. One of the membrane separation technology for ILs recovery from aqueous solutions can be electrodialysis (ED). Thus, the objective of this study was to examine the efficiency of electrodialytic [BBIM]Cl recovery from wastewater, as well as the chemical stability of the recovered IL. Moreover, the characteristics of the tested ion-exchange membranes (IEMs) before and after ED were deteremined.

The [BBIM]Cl recovery from model aqueous wastewater was carried out using an EDR-Z/10-0.8 module (MemBrain, Czech Republic) with an effective single membrane area of 64 cm^2. There were 5 pairs of the IEMs. The IEMs used in this study were the AMA – AMC (Ionsep, China) and AM(H) – CM(H) (Ralex, Czech Republic). The concentrations of the [BBIM]Cl in experimental solutions were determined by using a UV-VIS

spectrophotometer (Shimadzu UV-2700i, Japan). The surface morphology of the tested IEMs before and after ED were investigated by using a scanning electron microscope (SEM, FlexSEM 1000 II VP-SEM, Hitachi, Japan), and by an atomic force microscopy (AFM, CoreAFM Nanosurf). Moreover, the chemical composition of the tested IEMs were examined by the attenuated total reflection-Fourier transform infrared spectroscopy. The chemical stability of the recovered [BBIM]Cl was determined by Nuclear Magnetic Resonance (NMR) method.

It was found, that the ED allows for the effective [BBIM]Cl recovery from aqueous solutions. Moreover, the surface morphology of the IEMS after ED was not differ significantly in comparison to the pristine IEMs. In addition, the FTIR–ATR spectra of the tested membranes confirmed no significant change in the chemical composition of the IEMs after electrodialytic [BBIM]Cl recovery. It was confirmed that the recovered [BBIM]Cl had the same structure as the fresh solution of [BBIM]Cl. Therefore, it could be concluded that the recovered [BBIM]Cl was stable and could be reused.

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ENVIRONMENTAL PROTECTION TECHNOLOGY

POSTERS

WATER QUALITY IMPROVEMENT VIA CALCIUM CARBONATE RECOVERY FROM BOREHOLE WATER IN ZANGO AREA OF LOKOJA, KOGI STATE, NIGERIA

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This study investigates the effectiveness of thermal treatment in improving the quality of borehole water in Zango through the recovery of precipitates. The study area was divided into two sections (Upper and Down Zango). Borehole water samples were subjected to boiling, and subsequent analyses were performed to evaluate changes in physicochemical parameters, metal concentrations, and mineral composition. The results indicated significant alterations to the physicochemical parameters due to thermal treatment. Atomic Absorption Spectroscopy (AAS) results showed a significant decrease in the calcium ion concentration from 28.339 ppm in RwUp to 8.419 ppm in Raw Water from Down Zango (TwUp), and from 116.090 ppm in Raw Water from Up Zango (RwDown) to 12.970 ppm in TwDown, highlighting the treatment's impact on metal removal. X-ray Diffraction (XRD) analysis identified aragonite as the major mineral phase, with 92% purity in the precipitate in Precipitate from Up-Zango Up-Zango (Pa) and 89% purity in the precipitate in Precipitate from Down-Zango (Pb). The minor mineral phases in Pa and Pb were siderophyllite (8%) and annite (11%), respectively. X-ray Fluorescence (XRF) results confirmed a high concentration of calcium oxide, at 88.119% in Pa and 82.269% in Pb. Both the XRD and XRF results support the effectiveness of thermal treatment in precipitating calcium-based minerals in water. These findings demonstrate that thermal treatment not only enhances water quality by reducing hardness and contaminants but also alters the mineral composition of the precipitate. The study provides valuable insights into the practical application of thermal methods for water purification and the recovery of valuable minerals, contributing to improved water management practices in regions with similar geological and environmental conditions.

The authors acknowledge the financial support from the Slovak Society of Chemical Engineering

HYDROXYLATION AS THE VERY FIRST STEP DURING HETEROGENEOUS PHOTOCATALYSIS OF AZO DYES

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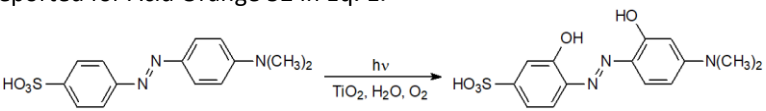
Azo dyestuffs account for 60-70 % of the total 700,000 t/year world production of organic dyes. They represent environmental problem due to waste waters coming from dyeing processes. Methods for their remediation have attracted increasing attention in the field of environmental technology development. One such a method is heterogeneous photolysis, in which organic pollutants are oxidized either by photogenerated positive holes (h^+) or by reactive oxygen species (•OH) formed under irradiation on the catalyst surface. The attack of •OH radical as a first step for the photocatalyst induced process is well established. The formation of stable hydroxylated intermediates has also been earlier reported for Acid Orange 52 in Eq. 1.



(1)

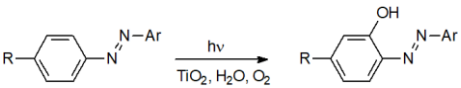
The aim of this work was to advance our understanding of the structure of primary reaction products and their influence on the absorption spectra during aerobic heterogeneous photolysis of commercial azo dyes Acid Orange 7 (AO7) and Reactive Red 2 (RR2).

AO7 and RR2 were photocatalytically degraded in a titanium dioxide slurry. Reaction products of AO7 were analyzed by NMR and MS spectroscopy as well as HPLC.

A previously undescribed primary intermediate, 3-hydroxy-4-[(2-hydroxy-1-naphthyl)diazenyl]benzenesulfonic acid, originated from AO7 was detected and isolated on a preparative scale from the photoreactor. The identity of the photolysis product was confirmed by comparison with a chemically synthesized standard.

We found that the primary process in the heterogeneous photolysis of AO7 is a mono-hydroxylation reaction on the benzene ring at a position adjacent to the azo group. The same pattern of heterogeneous photolysis we observed also for RR2.

So we concluded reaction model in Eq. 2 is very probable for the broad group of di-aryl azo dyes following general formula in Eq. 2.



(2)

The support from the Faculty of Chemical Technology, University of Pardubice, the Czech Republic, is gratefully acknowledged.

VALIDATION OF CATALYTIC BIOGAS AND OFF-GAS METHANATION: PILOT TESTING UNDER REAL CONDITIONS AT A WASTEWATER TREATMENT PLANT

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Power-to-Gas (P2G) technology in the sense of producing methane-rich gas by reacting carbon dioxide and hydrogen can be based on one of two principles. The first is the biological route, whereby the conversion (hydrogenation of carbon dioxide) occurs with the help of methanogenic bacteria at temperatures around 60 °C and pressures close to atmospheric pressure. This approach is being pursued by many research institutions, however no equipment has yet been implemented or verified on a semi-operational scale in the Czech Republic. The second principle is a chemical pathway based on a catalytic reaction taking place at temperatures of 200 - 400 °C and pressures in the order of units of MPa. In the literature, a higher process in tensity is cited as a major advantage of chemical conversion, as a result of which plants of comparable performance can be significantly smaller. This can be illustrated by a number of examples of pilot plants operating mainly in Germany or Switzerland, Denmark and Italy. From the available public sources, there is no company in the Czech Republic that has its own P2G technology solution, nor has such a device been tested in the Czech Republic on a pilot or semi-operational scale. For this reason, the unique equipment (methanation unit) will be developed and connected with a real biogas source. In the second phase an existing CO2 source from biogas upgrading will be utilized at the central wastewater treatment plant (WWTP) in Prague. Existing biogas upgrade is based on CO2 separation using membrane technology, with no further utilization of carbon dioxide to potentially increase biomethane/renewable natural gas (RNG) production. Development and verification of P2G technology for producing RNG enables partial substitution of natural gas in the distribution network. The goal is to reduce the carbon footprint of natural gas and utilize waste CO_2 from biogas upgrade at WWTP. The project combines laboratory research (nowel catalyst development and its optimization) with development and testing directly central WWTP in Prague. In the final phase, the potential of industrial up-scale and optimal integration will be assesed and proposed. Initially, the technology will be adapted to meet legislative and WWTP internal requirements, then integrated on-site and tested alongside existing membrane separation.

ARE PYROLYSIS CHARS REALLY SAFE FOR ENVIRONMENTAL APPLICATIONS? AN ECOTOXICOLOGICAL PERSPECTIVE

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Pyrolysis is increasingly promoted as a promising technology for waste valorisation within the framework of circular economy and sustainable waste management. The resulting chars are frequently proposed for environmental applications, such as soil amendments or adsorbents for water treatment. However, most studies focus only on physicochemical characterization of these materials, while potential environmental and ecological risks remain insufficiently assessed.
In this study, chars produced from three different waste streams (biomass, waste tires, and electro-waste plastics) were comprehensively evaluated. In addition to physicochemical and surface characterization, the evaluation included analysis of polycyclic aromatic hydrocarbons, aqueous leachates, volatile organic compounds, and ecotoxicological tests using aquatic and terrestrial model organisms.
Results revealed substantial differences between the tested materials. All char leachates inhibited the growth of algae, with the strongest effect observed for char derived from electrowaste plastics. Similar trends were observed in tests with *Daphnia magna*, where electrowaste char leachates caused complete immobilization of organisms. In soil tests, the application of chars slightly reduced lettuce seed germination, particularly at higher doses of char from the electrowaste.
From a practical perspective, tire-derived char was unsuitable for soil application due to elevated PAHs concentrations exceeding legislative limits. Although its physicochemical properties suggested potential use as an adsorbent, increased toxicity to aquatic organisms was observed, probably related to the high salinity and alkalinity of its leachate. As a result, its potential application is more suitable for air purification systems. Char derived from electrowaste plastics showed the highest environmental risk, containing elevated concentrations of hazardous elements and VOCs, which excluded its use in environmental applications.
These findings demonstrate that conventional physicochemical characterization alone is insufficient to evaluate the environmental safety of chars. Therefore, the ecological assessment should be incorporated into the evaluation of waste-derived materials intended for environmental applications.

OZONATION AND ION PAIRING AS METHODS FOR PURIFICATION OF MODEL WATERS CONTAINING AZO DYES

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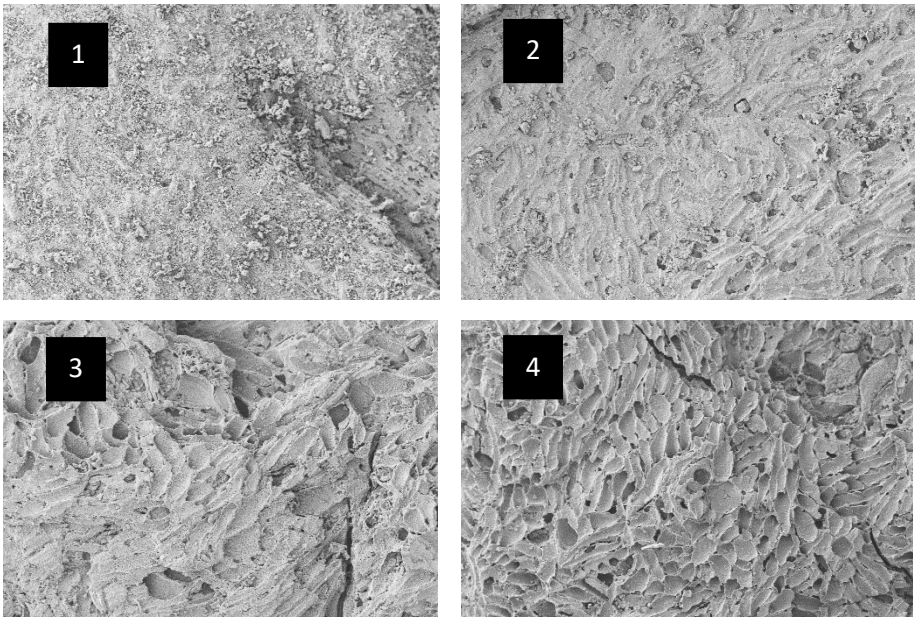
This work investigated the possibility of treatment of model and industrial wastewater contaminated with selected textile azo dyes. Two methods were used: ion pairing using quaternary ammonium salts and subsequent filtration and, within the framework of AOP methods, ozonation, or ozonation catalyzed by carbonaceous materials. Biochar, granular activated carbon and, when appropriate, sludge, which was a product of textile industrial water treatment, were used as carbonaceous materials. Both their sorption and catalytic properties were compared, including the possible regeneration and reuse of the carbonaceous materials as sorption material and as a possible ozonation catalyst.



Pictures 1-4: Gradual decomposition of GAC due to ozone

ELECTROCHEMICAL COMPRESSION - ADVANCED HYDROGEN COMPRESSION TECHNOLOGY

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Hydrogen technologies are currently gaining importance due to their potential for more efficient use of electrical energy compared to conventional technologies and for converting or storing surplus energy from renewable energy sources (RES). In addition to fuel cell and water electrolyzer technologies, electrochemical hydrogen compression (EHC) technology is also available, offering higher efficiency compared to mechanical compressors, quiet operation without vibration, and higher reliability due to the absence of moving parts. In addition, this technology combines separation and compression properties, as only hydrogen is removed from the anode input mixture during the process. EHC can therefore also be used to produce high-purity hydrogen, the degree of contamination of which will be determined solely by the permeation characteristics of the membrane used and the tightness of the cell.

The role of hydrogen technologies in the zero-emission energy market is constantly growing. Hydrogen economies are being built both centrally and locally, close to where the energy will be used. As the amount of zero-emission hydrogen produced grows, dealing with low energy density is becoming more and more important. There are two ways to minimize the space requirements of storage capacities: compressing hydrogen to higher pressures or liquefying it. The hydrogen liquefaction process requires higher investment and operating costs and is therefore currently less common in applications ranging from units to tens of MW of installed power. However, the disadvantage of conventional mechanical hydrogen compressors is high noise levels, vibration, the risk of media contamination, and mechanical fatigue of materials.

The aim of the project is to research and develop effective methods of electrochemical hydrogen compression (EHC). In the first phase of the project, laboratory equipment based on a single EHC cell was designed, manufactured, and tested to verify the basic principle and standardize testing procedures. In the second phase, the research team is focusing on upscaling and designing a multi-cell stack, which, with its parameters (e.g., increasing the electrode area from units to tens), is approaching commercial use. In parallel, research and development of key sub-components, such as optimized membranes and ionomers, is underway with the aim of integrating experimental materials into the entire system and achieving maximum device performance.

VYUŽITÍ SYNERGICKÉHO EFEKTU SORPCE A FOTOKATALYTICKÉ OXIDACE PRO ODSTRAŇOVÁNÍ MIKROPOLUTANTŮ Z VOD

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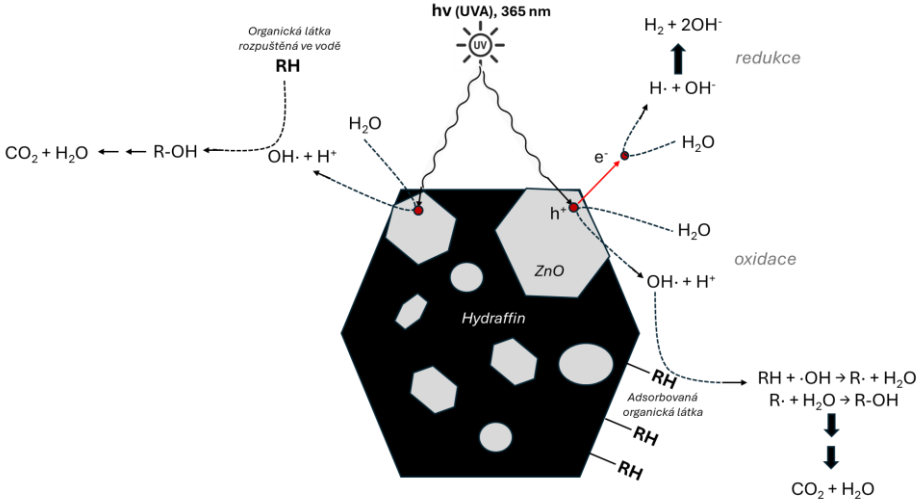
Mikropolutanty představují širokou skupinu organických xenobiotik, které se do vodního prostředí dostávají zejména z průmyslu, zemědělství a komunálních odpadních vod. Významnou část z nich tvoří pesticidy a léčiva, jež jsou do prostředí uvolňovány při zemědělské aplikaci nebo po spotřebě člověkem a jejich následném nedostatečném odstranění v čistírnách odpadních vod. Tyto látky se ve vodách vyskytují v nízkých koncentracích, avšak mohou být perzistentní, biologicky aktivní a potenciálně nebezpečné pro vodní ekosystémy i lidské zdraví.
Cílem této studie byl vývoj technologie využívající synergického efektu sorpce a katalytické fotooxidace pro efektivní odstranění mikropolutantů z vod. Principem navržené technologie je kombinace nově vyvinutého fotoreaktivního materiálu – uhlíkového sorbentu (hydraffin) modifikovaného fotokatalytickými nanočásticemi ZnO – a UV záření vhodné vlnové délky. Výsledkem je sorpčně-degradační proces, při němž dochází k zachycení mikropolutantů na sorbentu a jejich následné fotooxidaci, což umožňuje rychlé a účinné odstranění těchto látek z vod a současně dochází k prodloužení životnosti nově vyvinutého sorbentu oproti standardním formám sorbentů na bázi konvenčního aktivního uhlí.



Princip fotooxidčních reakcí při interakci UV záření s hydraffinem modifikovaným ZnO