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PLENARY LECTURES

CHEMICAL INDUSTRY TRANSITION PATHWAY – EU CHEMICAL INDUSTRY COMPETITIVENESS

I. Souček

Svaz chemického průmyslu ČR
VŠCHT, Praha

EU transition to carbon neutrality is dependent on several key aspects:

1. Profitability and sustainability of chemical industrial sector itself
2. Focusing on prioritised areas contributing to transition

The plenary paper describes current status of EU chemical industry competitiveness compared to other traditional chemical world regions (esp. USA and China).

Results of iC2050 modelling of EU chemical industry is presented based on "Carbon manager" presented by Cefic in 01/2025 highlighting 4 main areas of contribution (covered by appropriate legal frame):

- Circularity
- Digitalisation
- Safe and sustainable chemicals
- Climate neutrality

Despite the **electrification of processes**, the carbon plays an essential role for chemical industry. **Access to biomass** is indispensable in order to substitute fossil molecules. Although polymer waste and captured CO2 are important complementary solutions.

The **competitiveness** of the chemical industry will shape and influence the ability of the sector to achieve its transition. The sheer amount of capital and operational budget will need to be financed with higher revenues providing a return on investments. **Boosting demand for net zero, low carbon and circular products** is therefore essential. A fundamental assumption is the **fixed amount of production** happening in Europe: EU cannot achieve the climate and circularity objectives by closing down capacity and replacing with imports. The reality is different: failing to create the necessary enabling conditions for the chemical sector's transition, will not only weaken climate action but also potentially lead to a deterioration of the EU's economic fabric.

The transition of the Czech chemical industry to carbon neutrality by 2050 is associated with:

1. **For the deployment of abatement solutions, achievement of carbon neutrality requires investments between EUR 17.2 – 28,8 billion by 2050**
2. **The industry electricity consumption for the defined part of the sector will gradually increase from 1.5 TWh to 5 - 12 TWh (depending on the selected sub-scenario).**
3. **The total biomass demand is about 1 million t/year in the last decade of the period under review.**
4. **Over this period out of CO_2 will be emitted, 3.3-8.7 mil. t/y of CO_2 will be captured (of which 2.6-8.5 mil. t/y of CO_2 will be stored (CCS) and 0.2-0.7 mil. t/y of CO_2 will be used (CCU))**

ENERGY CONVERSION AS A UNIFYING TOPIC OF ECONOMY DECARBONISATION

K. Bouzek

Department of Inorganic Technology, University of Chemistry and Technology, Prague, Technicka 5, 166 28 Prague 6, Czech Republic

Decarbonisation of economy of the industrially developed countries represents widely discussed topic. Usually it is connected exclusivelly with reduction of CO_2 emmissions. Additional, at probably even more important aspect represents diversification of energy and raw materials sources. Conversion to the renewable sources represents significant contribution to this policy. Increasin importance of this aspect we could follow with increasing intensity for the decades. Extreemely visible it become after the start of the war on Ukraine.

Economy decarbonisation represents very complex problem related to numerous aspects of energetics, transportation and industry. Unfortunatelly, it is usually seen just in connection with separated particular problems, like potential ban on the cars propelled by combustrion engines. Analogously, also research sphere is divided to the individual groups dealing with particular aspects related to their domain of interest. It often happens withou connection to the broader framework. At the same time, it is obvious, that without interdisciplinar communication and collaboration all research and developemt effort will be significantly more demanding and importantly more dificult to transfer to dailly life applications. The target of this contribution is to introduce a trial to interconnect individual fields involved in this research crucial for the future of human society.

The project „Energy conversion and storage“ was proposed to address most important technologies in the field of renewable energy production and integration into our daily lifes. It focuses on three main approaches to energy conversion represented by: (i) solar energy conversion o the electrical one, or to the energy of chemical bond, (ii) conversion of electrical energy to the energy of chemical bond (mainly hydrogen as an energy vector and e-fuels) and (iii) batteries and supercapacitors. Research and development in each of these fields is supported by the three cross cutting activities providing cutting edge methodologies needed for efficient work and future transfer of results achieved to the daily life pracice, namely: (a) molecular design, (b) engineering and (c) energetics – buildings, cities and communities.

As it is clearly visible, the problems is handled in a broad perspective of most of the involded research field. Its target is to established highly qualified plaform allowing to generate high quality inerdisciplinar research projects (including commercial ones) and provide one point highly qualified contact for the field of energy conversion and storage for commercial sphere, as well as for public administration.

This work was supported by the project "The Energy Conversion and Storage", funded as project No. CZ.02.01.01/00/22_008/0004617 by Programme Johannes Amos Comenius, call Excellent Research.

HYDROGEN A TOOL FOR DECARBONIZATION OF CHEMICAL INDUSTRY

P. Mervart

Ministry of Industry and Trade, Prague

The European Commission has set mandatory targets for replacing hydrogen in the chemical industry with renewable hydrogen, presenting significant challenges for the Czech chemical sector. In line with the Czech Hydrogen Strategy, the proposed solution focuses on expanding renewable hydrogen production and repurposing existing natural gas pipelines for hydrogen transport. To support this transition, the Ministry of Industry and Trade is implementing various measures to establish a legal framework for renewable hydrogen use and lower production costs.

SELÉN – JEDOVATÝ, ESENCIÁLNY ČI LIEČIVÝ?

V. Milata

Ústav organckej chémie, katalýzy a petrochémie, Fakulta chemickej a potravinárskej technológie, Slovenská technická univerzita, SK-812 37 Bratislava, Radlinského 9

Selén je esenciálny prvok, ktorý bol objavený Jönsom Jacobom Berzeliusom vo švédskych meďnatých pyritoch v roku 1817. Na druhej strane je to prvok, ktorého prchavé či rozpustné zlúčeniny sú jedovaté. Svojou povahou je kov či polokov tvoriaci prechod medzi telúrom a sírou či arzénom a brómom v periodickej tabuľke prvkov.

Nedostatok selénu spôsobuje Keshanovu chorobu, či u detí chorobu Kashin-beck (endemická choroba kostí najmä v oblasti Číny), ktoré spôsobujú napríklad poruchy v metabolizme selenoproteínov.

Tieto vlastnosti dávajú dobré predpoklady pre vývoj organoselénových zlúčenín aplikovateľných v humánnej alebo veterinárnej terapii. Preto sme pripravili niektoré typy zlúčenín selénu a ich výsledky budeme prezntovať na prednáške.

Tento príspevok vznikol vďaka podpore v rámci Operačného programu Integrovaná infraštruktúra pre projekt: „Strategický výskum v oblasti SMART monitorovania, liečby a preventívnej ochrany pred koronavírusom (SARS-CoV-2)“, Projekt č. 313011ASS8, spolufinancovaný Európskym regionálnym rozvojom a Agentúrou pre podporu výskumu a vývoja na základe zmlúv č. APVV-20-0213 a VEGA 1/0385/25.

MATERIALS ENGINEERING

LECTURES

OPTIMIZATION OF THE PREPARATION OF IRON SILICIDE – NICKEL ALUMINIDE COMPOSITE

P. Novák, S. Mestek, J. Duda, A. Michalcová, F. Průša

University of Chemistry and Technology, Prague, Department of Metals and Corrosion Engineering, Technická 5, 166 28 Prague 6, Czech Republic

Composite consisting of a NiAl matrix and FeSi reinforcement is being developed as a hard and wear-resistant material that could potentially replace cemented carbides or some tool steels. In its current form, its tribological properties are comparable to common cold-work tool steels, but its advantage is that it does not require heat treatment in the form of quenching and tempering to achieve them. Previous research showed that the homogenization of FeSi and NiAl phases is a crucial step for achieving good mechanical properties. Therefore, this work focuses on optimization of preparation of iron silicide and nickel aluminide and their homogenization by high-energy ball milling.

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

AS-CAST AL-CO ALLOYS: MICROSTRUCTURE, PHASE CONSTITUTION, AND CORROSION BEHAVIOR

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Aluminum alloys are lightweight structural materials with wide applications in the automotive, aviation and food industries. The alloys, however, can also be used as anodes in Al-air batteries to produce electricity from the reaction of oxygen in the air with Al. Furthermore, the reaction of Al with water can be utilized to produce hydrogen. The reaction is enhanced under alkaline conditions. In this work, the phase constitution, microstructure, and corrosion behavior of Al alloys with 1 and 3 at. % Co were studied. The results were compared with pure Al. Al-1%Co and Al-3%Co alloys were prepared by arc melting of high purity Al and Co lumps in argon. Subsequently, the alloys were rapidly solidified to form cast strips. The as-cast Al-1%Co alloy had a near-eutectic microstructure. The eutectic consisted of thin lamellae of the Al_9Co_2 phase and a solid solution of Al. The Al-3%Co alloy had a hypereutectic microstructure consisting of a dendritic, primarily precipitated Al_9Co_2 phase and a eutectic. The corrosion behavior of the alloys was investigated by open circuit potential measurements, linear sweep voltammetry and hydrogen evolution experiments. Corrosion resistance was studied in a dilute NaOH solution (0.01 mol dm^{-3}) at room temperature. During corrosion, a preferential dissolution of the eutectic has been found. The primary dendritic Al_9Co_2 phase in the Al-3%Co alloy was significantly less affected and served as a microcathode during corrosion. The dendrides of the primary Al_9Co_2 phase remained covered with an adhesive layer of corrosion products during immersion in the NaOH solution. The corrosion of the alloys was found to be significantly enhanced compared to that of pure Al. The results of the study can be used for the practical design of Al alloys for on-board production of H_2.

This work was funded by the Slovak Research and Development Agency (project no. APVV-20–0124), the Scientific Grant Agency of the Ministry of Education, Science, Research and Sports of the Slovak Republic and the Slovak Academy of Sciences VEGA (projects nos. 1/0692/22 and 1/0531/22) and the NextGenerationEU recovery package of the European Commission through the Recovery and Resilience Plan for Slovakia under the project No. 09I04-03-V02-00046.

BIOMASS ASH: A STUDY OF ITS LEACHABILITY

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In recent years, the energy sector has been preparing for a transition from coal combustion to purely ecological green energy sources. This brings changes that have and will have a significant impact on the construction industry. One of these green energy sources is biomass. Biomass ashes generally have a high content of chlorides, sulphates and alkalis, which complicates their use in the construction industry. From a legislative perspective, BMA ash is classified as waste.
This study focuses on the leachability of 51 BMA ash samples from six locations in the Czech Republic, produced from grate and fluidized bed combustion of biomass and co-combustion of biomass with coal. The main emphasis was placed on the leachability of heavy metals and other potentially dangerous chemical substances. Simultaneously, pH, electrical conductivity (EC), total dissolved solids (TDS), soluble inorganic salts (SIS), and dissolved organic carbon (DOC) were measured. It was found that most of the BMA ashes exceed the limits for TDS, chlorides, fluorides, sulphates, chromium, molybdenum, and selenium. Additionally, most of the samples showed excessively high pH and electrical conductivity.

This work was supported by the Technology Agency of the Czech Republic in the program Sigma with no. TQ03000837, 2024 – 2025.

INFLUENCE OF THE ADDITION OF MUNICIPAL WASTE ASH ON THE CARBONATATION IN CEMENT MORTARS

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Carbonation is a process in which atmospheric carbon dioxide reacts with calcium hydroxide in concrete, forming calcium carbonate. This process degreases the pH of the concrete, which can lead to corrosion of the steel reinforcement and thus endanger the durability of concrete structures. The rate of carbonation is influenced by the permeability of the concrete, humidity, and the concentration of CO_2 in the environment. Although concrete carbonation is generally considered a negative phenomenon, it contributes to reducing the concentration of CO_2 in the atmosphere. In this work, the effect of ash from the co-combustion of selected municipal waste with coal and limestone (fly and bottom MFBC ash) on the carbonation of mortar specimens was investigated. The reference samples were specimens containing standardized power plant fly ash and specimens prepared without admixtures, containing only Portland cement 42.5 R. Mortars with binder, standardized sand and water coefficient of 0.35 were prepared. Carbonation of the mortar specimens took place in an incubator under conditions of 3% CO_2, a temperature of 30°C, and humidity of 60-65%. The depth of carbonation was measured directly using the phenolphthalein test (PT) and indirectly by measuring compressive strength. The samples were tested after 7, 14, and 28 days. The results showed that mortars with MFBC ash exhibited faster carbonation than the mortar with cement only. The carbonation rate of mortars with MFBC ash did not exceed the carbonation rate of cement with standardized fly ash. In the mortars with ashes, carbonation was slowest in the sample of fly MFBC ash. The results from the compressive strength measurements did not clearly prove the effect of carbonation on the strength of the specimens.

This project was co-financed by the Technology Agency of the Czech Republic within the scope of THÉTA Program TK05020140 and from the grant of Specific university research – grants No. A1_FCHT_2025_009 and A2_FCHT_2025_054.

JOURNEY TO LONGER TOOL LIFE: $AL_{0,67}TI_{0,33}N$ HARD THIN FILMS PREPARED BY ARC EVAPORATION

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Arc evaporation is a common method for deposition of very hard nitride thin films. In modern times, many ways to further evolve this method had been explored, and coatings with wide range of application fields were invented to suit requirements of modern industry. One of the most lucrative application is deposition of aluminium and titanium based nitride and carbonitride coatings with high hardness, wear and temperature resistance, enhancing the durability and lifespan of frequently used high speed steels and cemented carbides.

This study delves into preparation of aluminium-titanium based nitride and carbonitride thin films with metallic ratio of Al:Ti set at 67:33 at.%. Deposition was done by cathodic arc evaporation in HTC650 and HTC850 coating equipment from Hauzer Techno Coating. As target material has been chosen aluminium titanium alloy with mentioned atomic ratio of 67:33. Dependence of coating properties on temperature, substrate bias, arc current, rotation speed and multiaxial movement were investigated. Phase composition was analysed using Grazing incidence X-ray diffraction. Microstructure and macroparticle analysis were done by both scanning electron and confocal microscope, while roughness was determined by mechanical profilometer as well as by optical analysis. Adhesion on substrate was evaluated by Daimler-Benz and scratch tests. As for mechanical properties, their evaluation was done by microhardness measurement and wear rate reciprocating test.

As a one of the main results of this study, cubic and hexagonal coatings exhibiting very high hardness and different preferential crystal planes were deposited on both cemented carbides and high strength steel. Highest hardness above 33 GPa was acquired by pure cubic thin film with dominant (111) orientation. On the other hand, the best wear resistance of $5 \cdot 10^{-6}$ $mm^3 N^{-1} m^{-1}$ was exhibited by cubic thin film with dominant (200) orientation, indicating that crystallographic orientation plays a pivotal role in resulting properties.

This work was supported from the grant of Specific university research – grant No A2_FCHT_2025_079.

BINARY PHOSPHATE GLASSES – PREPARATION AND DISSOLUTION

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Phosphate glasses have attracted significant interest over the past few decades due to their remarkable properties, particularly their solubility, which makes them ideal for biomaterial applications. Their chemical durability, along with other characteristics, can be tailored for specific applications, making phosphate glass a versatile material. However, the preparation of phosphate glasses can be challenging. Phosphate melts are often corrosive to most conventional crucible materials, which can introduce impurities into the glass. Additionally, some phosphate glasses are prone to crystallization during preparation. These issues contribute to the limited research on phosphate glasses, especially simpler, high-phosphate-content compositions.

For phosphate glass-based (bio)material applications, multicomponent glass compositions are typically chosen.[1] However, to understand the impact of composition on dissolution behaviour, it is crucial to differentiate the effects of each component. This can be studied using simple, binary phosphate glasses. Moreover, simple glass systems allow for the investigation of impurity effects on the dissolution process.

This study aims to explore the effects of modifier cations in binary phosphate glass compositions on dissolution behaviour and to link these effects with the structural characteristics. Three series of binary phosphate glasses were prepared, each containing an alkaline earth cation (Ca^{2+}, Mg^{2+}, Sr^{2+}) as a modifier, with the content of the respective oxide ranging from 45 to 60 mol%. Glasses were prepared using a melt-quenching technique. Each series was prepared using different crucible materials (silica, alumina, platinum). The compositions of the glasses were analyzed by XRF, and the glassy state of all samples was confirmed by XRD. Static dissolution studies were performed using deionized water as the dissolution medium. The concentration of leached components in the leachates was measured using ICP-OES. Dissolution kinetics was calculated from the concentration data, and the results were compared with dissolution models.[2] Structural analysis of the glasses was conducted using ^{31}P solid-state NMR and Raman spectroscopy.

Acknowledgement:

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References:

[1] ABOU NEEL, Ensanya A., David M. PICKUP, Sabeel P. VALAPPIL, Robert J. NEWPORT and Jonathan C. KNOWLES. Bioactive functional materials: a perspective on phosphate-based glasses. *J. Mater. Chem.* [online]. 2009, **19**(6), 690–701. ISSN 0959-9428, 1364-5501.

[2] HELEBRANT, Aleš. Kinetics of corrosion of silicate glasses in aqueous solutions. *Ceramics – Silikáty*. 1997, **41**(4), 147–151

HIGH-TEMPERATURE RESISTANT HIGH-ENTROPY MATERIALS FOR THERMAL CIRCUIT COMPONENTS

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The energy sector is increasingly constrained by the limitations of conventional materials and manufacturing technologies. Highly stressed components, such as superheaters and turbine blades, face challenges related to insufficient mechanical properties and corrosion resistance, leading to reduced efficiency and shorter lifespans. Additionally, emerging applications, including high-temperature nitrogen cycles and industrial hydrogen production, are hindered by the lack of materials capable of withstanding extreme conditions. This project focuses on developing advanced materials to enhance the reliability and performance of thermal circuit components in such demanding environments. The primary objective is to create materials that exhibit exceptional high-temperature performance when exposed to extreme environments, such as supercritical water and nitrogen.

Currently, energy system components are predominantly manufactured using conventional techniques such as forging, casting, and mechanical machining, relying on standard materials like steel and widely available nickel-based alloys. However, these materials are approaching their performance limits, necessitating the development of advanced alternatives.

High-entropy alloys (HEAs) in particular hold significant promise for energy applications due to their combination of high strength and plasticity. However, even the most promising thermally stable HEA candidates often degrade rapidly in environments with residual oxygen concentrations. This project aims to develop a new class of HEAs that exhibit both superior thermal stability and oxidation resistance, making them suitable for demanding applications such as nuclear reactor cores and high-temperature energy systems. Despite progress in HEA development, immediate industrial deployment remains challenging due to the need for further optimization of alloy compositions and scalable production methods. To address this, several types of HEAs, including refractory high-entropy alloys (RHEAs), were prepared and tested to determine their mechanical properties and resistance to elevated temperatures in various environments.

This research was supported by the Technology Agency of the Czech Republic under project no. TK04020056 (High-temperature resistant materials for thermal circuit components).

HIGH-POWER MICROWAVE PLASMA GASIFICATION AS A CARBON SOURCE FOR COCRFENIMN ALLOY REINFORCEMENT

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High-power microwave plasma gasification (MPG) is one of the processing options for non-biodegradable polypropylene waste. In addition to syngas, the primary product of gasification, a nanostructured carbon by-product is also generated. Due to its large specific surface area, this MPG carbon shows potential for reinforcing metallic materials, which are typically strengthened through in-situ carbon reactions or the addition of pre-formed carbide particles. However, depending on the gasification process, the by-product is not pure carbon but contains small amounts of catalytic elements. The aim of this study was to assess the feasibility of producing carbide particles from MPG carbon and their potential use as reinforcement for the CoCrFeNiMn alloy.

Based on the optimization, suitable parameters of the mechanical alloying were selected for the preparation of the carbide particles from MPG carbon. Through the mechanical milling, the carbides were evenly distributed in the CoCrFeNiMn alloy, which resulted in enhancement of the mechanical properties. The chemical and phase composition of the prepared materials was analysed with XRF and XRD. Microstructure was observed with OM and SEM. Mechanical properties comprised the hardness and compressive tests of the prepared composites.

This work was financially supported by the Czech Science Foundation (project No. 24-10767S, Advanced high-entropy alloys reinforced by in-situ grown carbides formed from various types of nanostructured carbon precursors).

MATERIALS ENGINEERING

POSTERS

FREEZE-THAW DURABILITY OF CEMENT MORTARS WITH CO-COMBUSTION MUNICIPAL WASTE ASH

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The aim of this research was to investigate the possible use of ash produced from the co-combustion of coal with sorted municipal waste and limestone as a material with potential hydraulic properties. The obtained municipal FBC bottom ash (MFBC bottom ash) was treated by grinding in a ball mill. The research focused on the preparation and durability of mixed cement mortars to freeze-thaw. Specifically, the corrosion behaviour of mortars prepared with different percentages of cement replacement by MFBC bottom ash (10, 20, 30%) was monitored in the environment of frost, moisture and deicing salts. The results showed that bodies prepared from a mixture of MFBC bottom ash and cement displayed, according to the ČSN EN 72 1326, Z1 standard, better resistance to alternating freezing and thawing both in water and 3% NaCl environments compared to the reference Portland cement. Even with a high water to binder ratio w=0.5, the mixed mortars had an undisturbed or slightly disturbed surface after 100 freezing cycles. These results are very positive from the point of view of the use of MFBC bottom ash in construction, because data from the literature indicate significantly worse results even with a lower substitution of similar ash for cement.

This project was co-financed by the Technology Agency of the Czech Republic within the scope of THÉTA Program TK05020140 and from the grants of Specific university research – grants No. A1_FCHT_2025_009 and A2_FCHT_2025_054.

PLASMA TREATMENT OF VARIOUS METAL OXIDES: THE PATHWAY TO PREPARING NANOPARTICLES

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Plasma treatment is a highly effective technique for optimizing the morphology of powdered metal oxides, enabling precise control over particle size and shape. By exposing these materials to high-energy plasma, particles can be melted and rapidly solidified into uniform spherical structures, improving their flowability, packing density, and processability. Additionally, thermal plasma processing can fragment larger particles, allowing for a controlled reduction in size down to nanometers. A key objective of this study is to achieve particle sizes in the nanometer range, as plasma treatment provides a pathway to generating high-purity nanoparticles with tailored properties. This approach not only enhances material uniformity but also enables the scalable production of nanoparticles for advanced applications.

Nanoparticles of metal oxides exhibit superior functional properties compared to their bulk counterparts. Their increased surface area enhances catalytic activity, adsorption efficiency, and electronic performance, making them ideal for applications in energy storage, environmental remediation, and advanced coatings. The precise control over particle shape and size achieved through plasma processing further improves their mechanical properties, sintering behavior, and optical characteristics. This study demonstrates the feasibility of plasma-assisted nanoparticle synthesis and lays the foundation for future research aimed at refining plasma parameters to achieve even finer particle sizes, unlocking new potential in materials science and nanotechnology.

The financial support of the program "Strategy AV 21" of the Czech Academy of Sciences, specifically work package VP 27 Sustainable Energy (Renewable energy resources and distributed energy systems) are gratefully acknowledged

MICROSCOPIC CHARACTERIZATION OF NiAl/FeSi COMPOSITES

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The NiAl/FeSi composite samples were characterized by SEM and TEM microscopy. These materials composed of two separate phases and detailed observation enable us to observe the phase boundaries and crystallographic orientation of phases.

A detailed insight into the structure of these intermetallic materials will allow to describe the changes that take place in the microstructure during annealing, and ultimately the obtained results can help to find the optimal heat treatment regime to achieve the desired properties.

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CORROSION RESISTANCE OF 10 425 CSN/ S185 DIN PRESTRESSING STEEL REINFORCEMENT WITH BASALT COATINGS

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Corrosion damage to conventional prestressing steel reinforcement stimulated by chloride anions has caused a critical reduction in the load-bearing capacity and subsequent collapse of several major bridges and traffic structures in recent times. The use of appropriate protective coatings on the surface of prestressing reinforcement can provide a significant extension of the service life. This paper evaluates the barrier corrosion protection of a QAPF-classified basalt coating with high forsterite and diopside content when hot-dipped on conventional prestressing steel reinforcement by evaluating the porosity of the coating and exposure in 1 mol HCl and 3.5 wt. % NaCl solutions. The roughness (R_a) and phase composition (x-ray diffraction) of two variations of basalt coatings, namely those deposited at 1260°C on a preheated steel surface deposited by plasma spraying on a cold steel surface using a WSP-H 500 hybrid water-stabilized plasma torch, were also evaluated. The differences are noticeable mainly in the increase of the proportion of amorphous silica phases, which ensure almost zero porosity of the coating and high adhesion bond even to the plain bar surface of the reinforcement. Subsequently, the bond strength of the coated reinforcements in normal strength concrete was evaluated (pull-out test).

This research was supported by the Czech Science Foundation under grant no. 24-12783S.

MONITORING THE IMMEDIATE INTERACTION OF GLASS MATERIALS IN DEMINERALIZED WATER

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Glass corrosion, influenced by factors such as pH, temperature, and solution composition, plays a key role in both utility glasses and special glasses. Evidence of glass corrosion can be observed even on a daily basis, such as surface degradation on dishwasher-cleaned glassware. The extent of corrosion ranges from slight surface matting to complete degradation of glass material. In all applications, it is essential to understand how glass interacts with a solution during the initial moments of exposure. This knowledge enables precise modifications of the chemical composition of glass to meet specific requirements. A key focus is the analysis of the chemical composition of eluates from the very beginning of the interaction, which can be effectively carried out using ICP-OES.

This work aims to study the immediate dissolution of four types of glass (bioactive, sodium, potassium, and phosphate glass) in grit form under static conditions in demineralized water. The concentrations of the elements in eluates were analysed using ICP-OES, and pH measurements were performed at laboratory temperature.

This study confirmed that glass reacts in an aqueous solution within the first minutes of interaction, demonstrating the rapid initiation of the glass/water reaction. To fully understand this interaction, it is essential to analyse the material itself which will later be complemented by SEM/EDS and XRD material analyses.

This work was supported from the grant of Specific university research – grant No A1:FCHT_2024_008.

MICROSTRUCTURE AND PROPERTIES OF NITINOL ALLOY REINFORCED WITH NI-TI INTERMETALLICS AND CARBIDES

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Nitinol is well known for its unique properties, such as the shape memory effect and superelasticity. It is widely used in the medical field, particularly for stents and bone fixations. In industry, Nitinol finds applications as a joining element, temperature sensor, actuator, and vibration damper.

This study investigates the effect of reinforcing intermetallic particles and carbides on the hardness, wear resistance, and microstructure of Nitinol. The samples were fabricated using direct energy deposition (DED) from powder feedstock. A pre-alloyed NiTi powder

was used as feedstock material. The Ni-Ti intermetallic particles were formed in situ during the 3D printing process, while carbide particles were added separately.

This research was supported by the Czech Science Foundation (project no. 25-15757S).

SEMI-IPN HYDROGELS FOR CHEMICAL DELIVERY: TAILORING TRANSPORT AND MECHANICAL PROPERTIES

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Polyvinyl alcohol (PVAl) hydrogels are versatile materials with applications across various fields, including biomedical engineering, water purification, food packaging, and sensor technology. The effectiveness of these applications strongly depends on the mechanical and transport properties of the hydrogels, making it essential to explore new ways to tailor their performance. One promising approach is the incorporation of semi-interpenetrating polymer networks (semi-IPNs), where a secondary polymer is physically embedded within the hydrogel matrix. This strategy allows for controlled modifications of the hydrogel's mechanical and transport properties.

This study investigates the impact of polyelectrolyte additives on the mechanical strength and transport properties of PVAl-based hydrogels, with a particular focus on the diffusion of dye molecules. Hydrogels were prepared by cyclic freezing and thawing. To enhance material properties, sodium polystyrene sulfonate was introduced into the hydrogel network. Oscillatory rheometry was used to evaluate mechanical properties, particularly through strain sweep tests, which define the material's linear viscoelastic region. Macroscopic diffusion experiments, utilizing methylene blue and rhodamine 6G as tracer molecules, were conducted to assess transport behavior in modified versus unmodified hydrogels.

The results demonstrate that the addition of polyelectrolytes primarily affects dye transport, while having minimal impact on mechanical integrity within a specific concentration range. These findings highlight the potential of polyelectrolyte-modified hydrogels for applications requiring precise control over molecular transport, including biomedical, environmental, and industrial uses.

This study was supported by Technology Agency of the Czech Republic, project No.: TQ15000057.

OPTIMIZATION OF MOLYBDENUM AND VANADIUM CARBIDE SYNTHESIS FOR CANTOR ALLOY-BASED COMPOSITE ALLOYS

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Since their discovery, high-entropy alloys have attracted significant interest from materials engineers due to their unique properties. Notably, the Cantor alloy (CoCrFeNiMn) offers very high ductility and relatively good corrosion resistance. However, its drawback is its low yield strength and tensile strength. These properties can be improved by preparing a composite material in which the matrix consists of the Cantor alloy, while transition metal carbides serve as reinforcement.

A potential way to reduce the cost of producing such a composite would be to utilize waste nanostructured carbon obtained from the microwave pyrolysis of hydrocarbons yielding syngas and the nanostructured waste C by-product. The waste carbon could then be utilized for a rapid synthesis of carbides via mechanical alloying.

The aim of this work was to optimize the synthesis of molybdenum and vanadium carbides using waste carbon from the microwave plasma pyrolysis of polypropylene. The carbides were prepared using the mechanical alloying method. The synthesized carbides were incorporated as reinforcement into a composite alloy with a Cantor alloy matrix. The study examined the effect of increasing the reinforcement content and the homogenization method of the composite on changes in its mechanical properties. The Vickers hardness, compressive yield strength, and tribological properties of the composite were evaluated.

This work was financially supported by the Czech Science Foundation (project No. 24-10767S, Advanced high-entropy alloys reinforced by in-situ grown carbides formed from various types of nanostructured carbon precursors).

INCORPORATION OF TIC INTO NITI ALLOYS FOR THE DEVELOPMENT OF ADVANCED BALLISTIC PROTECTION MATERIALS

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Advanced ballistic materials prioritize weight reduction, impact resistance, and energy dissipation. Standard armour combines steel, Al/Ti alloys, ceramics, and fiber-reinforced polymers, but ceramic degradation at high-velocity impacts remains a challenge. A promising alternative embeds ceramic particles in metal matrices with 1D/2D carbon structures (CNTs, graphene) for superior strength.

Plasma-catalytic pyrolysis enables the synthesis of carbide/nanostructured carbon nanocomposites using metal oxides such as TiO_2 or WO_3 under extreme thermal conditions. The resulting carbide-based materials could significantly enhance ballistic protection when integrated into NiTi alloys, offering high strength, toughness, and reduced density.

This work focused on the initial assessment of TiC particle incorporation into NiTi alloys, primarily optimizing cohesion through mechanical milling. Initial tests showed poor cohesion in the mixed materials making the compositions exceeding 12.5 wt.% TiC entirely unusable. Therefore, mechanical milling was employed, doubling the total amount of reinforcing particles while improving particle distribution and enhancing material performance in relation to milling duration.

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).

PLASMA ASSISTED SYNTHESIS OF MAGNESIUM AND ZINC-MODIFIED CESIUM LEAD BROMIDE

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Cesium lead bromide ($CsPbBr_3$) has emerged as a promising material for optoelectronic applications due to its outstanding luminescence properties, high quantum yield, and potential for use in radiation detection, light-emitting diodes (LEDs), and photovoltaic devices. Its excellent charge transport characteristics and stability make it a valuable candidate for next-generation scintillators and high-resolution imaging technologies. However, the intrinsic instability of $CsPbBr_3$, particularly its moisture sensitivity and phase separation, necessitates modification strategies to enhance its structural and optoelectronic properties.

In this study, we report a novel approach for the plasma-assisted synthesis of magnesium (Mg) and zinc (Zn)-modified $CsPbBr_3$. The use of thermal plasma enables rapid synthesis with high purity and tunable composition. The incorporation of Mg and Zn into the $CsPbBr_3$ host matrix leads to significant alterations in structural and luminescence properties. X-ray diffraction (XRD) analysis confirms phase stability, while electron paramagnetic resonance (EPR) and photoluminescence (PL) measurements reveal enhanced emission efficiency and extended carrier lifetimes. The modification with Mg and Zn suppresses defect states and improves radioluminescence performance, making these materials highly suitable for radiation detection and advanced optoelectronic applications. Our findings demonstrate that plasma-assisted synthesis is an efficient and scalable route for tailoring the properties of $CsPbBr_3$-based materials, paving the way for their practical implementation in high-performance devices.

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PROCESS ENGINEERING

LECTURES

NOVÉ TECHNOLOGIE PROCESNÍ NIR A RAMANOVY SPEKTROMETRIE V CHEMICKÉM PRŮMYSLU.

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V rámci konference ICCT 2025 představíme nové technologie procesních spektroskopů pro procesní analýzu v chemickém průmyslu. Tyto technologie umožňují kontinuální monitorování v reálném čase, minimalizují potřebu vzorkování a poskytují okamžitou kontrolu kvality bez nutnosti složité přípravy vzorků.

Zaměříme se na jejich hlavní výhody, jako je zlepšení kontroly výrobních procesů, snížení provozních nákladů a optimalizace chemických reakcí.

Přednáška nabídne přehled nejnovějších trendů v této oblasti a jejich přínosu pro efektivnější, udržitelnější a konkurenceschopnější chemickou výrobu.

THERMAL PLASMA APPROACH FOR THE LARGE-SCALE PRODUCTION OF HYDROGEN AND CARBON AS WELL AS INORGANIC NANOPARTICLES

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Generation of thermal plasma implemented in the high-enthalpy chemical processes requires a specific facility – a device called plasma torch connected to a specific reactor. There are two operating modes utilized: pyrolysis and gasification. The pyrolysis mode is realized without adding an external oxidizing agent into the reactor. The gasification mode takes place when some oxidizing agent is used, e.g., CO_2. This also leads to the carbon utilization part in the carbon capture utilization and sequestration (CCUS) process. Hydrocarbons at the input can be valorized into synthesis gas (syngas), a valuable product on market for e.g., methanol or ethanol production. It is composed of hydrogen and carbon monoxide (the hydrogen content can reach 90%). Even pure hydrogen can be produced out of simple hydrocarbons containing only C-H-like bonds. Carbon nanoparticles (graphite or graphene) are synthesized in the same process as well. This can create a new sector in the market considering the high demand for carbon in relation to the production of batteries and supercapacitors.

The described technology may become crucial for the plastics upcycling, as starting from 2030 the storage of plastics is expected to be prohibited (https://www.europarl.europa.eu/news/en/press-room/20240419IPR20589/new-eu-rules-to-reduce-reuse-and-recycle-packaging).

Another important thermal plasma application is inorganic nanoparticles synthesis. It is worth noting that the plasma temperatures reach 10000-20000 ℃ depending on the gas (plasma medium) flow rate and power supplied to this gas. This is enough to produce inorganic nanoparticles at the level of kilograms per hour. Moreover, this can be the path for the new materials synthesis impossible using the classical methods.

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PROCESS ENGINEERING

LPOSTER

SAMPLE FILLING IN ROTATIONAL RHEOMETRY AND CONDITIONS OF RHEOLOGICAL MEASUREMENT AND THEIR EFFECT ON THE FREE FALL OF A SPHERICAL PARTICLE IN A NON-NEWTONIAN FLUID

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This study deals with the sample filling and conditions (air humidity content) of rheological measurement and their influence on the results of the numerical simulation of a free-falling spherical particle. A carboxymethyl cellulose CMC solution was chosen as a non-Newtonian, shear thinning fluid. For measuring the rheological properties of CMC solutions, a rotational rheometer HAAKE MARS I was employed. The measured data were fitted by power-law and Yasuda-Carreau models. Sample filling and conditions of rheological measurement can significantly influence the evaluation of the rheological properties (model parameters). The results show that the air humidity content during the rheological measurement has a more significant effect on evaluated model parameters than the overfilling of the sample. These changes in rheological model parameters can lead to numerical simulation results differences of tens of percents. The results of this study illustrate the importance of choosing the correct methodology and conditions of the rheological measurement corresponding to the expected conditions in hydrodynamic experiments.

INORGANIC TECHNOLOGY

LECTURES

INFLUENCE OF CALCIUM SULPHATE ON THE QUALITY OF NS FERTILIZERS

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A combination of intensive agricultural practices, increasing application of high-analysis fertilizers and tighter air quality regulations has led to increasing sulphur deficiency in soils.

Plants are able to take up sulphur as a soil nutrient in sulphate form. This can be supplied directly through atmospheric deposition and sulphate fertilizers, or via the oxidation of organic sulphur or elemental sulphur fertilizers.[1] Sulphates enter to the metabolism of plants already in the roots or they are transported to the leaves, where, together with nitrogen, participate in the formation of proteins. [2,3]

One of sulphates applied to granular fertilizers, that serve as a source of sulphur, is calcium sulphate. When it used as a fertilizer, it directly supplies sulphur and calcium to plants. Calcium sulphate introduced into soil as a chemically neutral salt doesn’t form concentrated solutions and its pH is almost neutral.[4]

Calcium sulphate is used, either completely or partially dehydrated $CaSO_4.2H_2O$ and $CaSO_4$ of natural or synthetic origin, including waste products. Depending on the type of calcium sulphate used, fertilizers are prepared using different technologies. As the production process changes, the quality of the fertilizer and the storage properties of the product also change.

REFERENCES

1. Fertilizer International, Number 522, May -June 2024
2. Fertilizer International, Number 497, July - August 2020
3. Fecenko J., Ložek O.: Výživa a hnojenie poľných plodín, SPU v Nitre, 2000
4. Zielewicz W., Sw˛edrzy´nska D., Sw˛edrzy´nski A., Grzebisz W., Goli´nski P.: The Influence of Calcium Sulfate and Different Doses of Potassium on the Soil Enzyme Activity and the Yield of the Sward with a Mixture of Alfalfa and Grasses. Agriculture 2022, 12, 475

PRODUCTION OF GRANULATE CALCIUM NITRATE

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As a part of laboratory research, limestone sources and their processing into calcium nitrate suspension were investigated. Searching for the possibility of precipitating impurities from this suspension without using a large amount of ammonia or other hydroxides. Optimizing the addition of ammonium nitrate so that calcium nitrate crystallizes from the metastable phase to the stable phase at the production plant as quick as possible. Research focused on finding a suitable substance that will ensure the non-stickiness of the granules during drying process. Granulation on different types of granulators and drying tests in different types of dryers. Drying tests at different temperatures and times.

Processing research data from the laboratory for the design of the modification of the existing production plant. Utilizing as many existing devices as possible and specifying the missing devices. Based on the existing devices, identifying the limiting device and adapting the entire process to this device (hourly production). Specifying the missing devices, their design and incorporation within the layout options in the production plant. Development of a design for a drying section for granulate, which would be located next to the existing plant and its connection to the production line. Development of an accurate energy and material balance for this production plant. Calculation of the economics of the plant for the production of calcium nitrate.

USE OF ZEOLITE DUST IN THE PRODUCTION OF GRANULATED ZEOLITE

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Natural zeolite is a mineral with a crystalline structure, primarily composed of silicon and aluminium. The physicochemical properties of zeolites are key factor that make them highly versatile and suitable for various applications. Natural and surface-modified zeolites can effectively retain water and nutrients within their porous structures. Consequently, the application of zeolite can improve water and nutrient use efficiency in agricultural activities, thereby reducing the potential for surface and groundwater contamination.[1,2] Better utilisation of nutrients from fertilisers gives higher yields and reduces nutrient dispersion in the environment.[3]

This paper presents the results of laboratory, pilot-scale, and full-scale research on the production of granulated zeolite while achieving the desired properties of an environmentally friendly product. The primary raw materials used were two samples of zeolite dust. One sample contained clinoptilolite-Ca as the main component, while the other sample's main component was heulandite-Ca.

The aim of the research is to promote the use of natural materials in agriculture with a focus on sustainability and to minimize the use of chemicals or other materials whose synthesis processes may have a polluting effect on the environment.

REFERENCES

1. N. Grifasi, B. Ziantoni, D. Fino, M. Piumetti: Fundamental properties and sustainable applications of the natural zeolite clinoptilolite, Sustainable Waste Management & Valorisation within the Circular Economy Era, Environmental Science and Pollution Research, May, 2024
2. C. Sangeetha and P. Baskar. Zeolite and its potential uses in agriculture: A critical review, Agricultural Reviews, 37 (2) 2016: 101-108
3. R. Jarosz, J. Szerement, K. Gondek, M. Mierzwa-Hersztek: The use of zeolites as an addition to fertilisers – A review, Catena, Volume 213, June 2022

EFFECT OF PHOSPHORIC ACID ON THE QUALITY OF MODIFIED TANNATE COATINGS

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Úvod

Tanátové povlaky vznikajú reakciou skorodovaného železného predmetu s tanátovacím roztokom, čoho výsledkom je vznik fragmentovanej morfológie tanátu železitého na povrchu. Kvôli zlepšeniu ochranných vlastností sa pH tanátovacieho roztoku upravuje kyselinou fosforečnou (H_3PO_4) na hodnotu 2-2,5, čím vznikajú na povrchu fosforečnany železité, ktoré zvyšujú koróznu odolnosť. V tomto projekte sa k tanátovaciemu roztoku pridáva hydrotalkit spolu s kyselinou fosforečnou a sleduje sa vplyv kyseliny fosforečnej na kvalitu modifikovaných tanátových povlakov.

Metodika

Modifikovaný tanátový povlak s prídavkom H_3PO_4 sa nanášal technikou ponoru. Po predúpravných operáciách sa povlak aplikoval v dvoch vrstvách. Pripravené vzorky sa charakterizovali pomocou EDX, SEM, XRD a elektrochemických meraní. Elektrochemické charakteristiky z LSV meraní sa získali v ASTM elektrolyte po stabilizácii OCP po dobu 40 min s trojelektródovým zapojením.

Výsledky

Porovnaním vzoriek bez a s pridaním H_3PO_4 sú pozorované zmeny v morfológii, EDX aj XRD záznamoch. Po úprave pH tanátovacieho roztoku obsahujúceho hydrotalkity sa pomocou XRD analýzy potvrdilo, že došlo ku chemickej reakcii medzi H_3PO_4 a hydrotalkitmi. Výsledkom tejto reakcie je rozklad hydrotalkitov a vznik nových fáz. Výsledky elektrochemických meraní slúžia na zhodnotenie vplyv účinku H_3PO_4 na kvalitu modifikovaného tanátového povlaku.

Záver

Na základe meraní sa zistilo, že vplyv kyseliny fosforečnej na modifikovaný tanátový povlak je zásadný ako z hľadiska charakterizácie povlaku pomocou analytických techník, tak aj na základe získaných elektrochemických charakteristík.

Táto práca vznikla vďaka podpore MŠVVaŠ SR v rámci projektu VEGA 1/0436/23.

ZPLYŇOVÁNÍ OLEJŮ V TECHNOLOGII MSG

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Centrum výzkumu Řež, Husinec-Řež, Česká republika

Úvod

Zplyňování je technologický proces známý již od poloviny 19. století. Společně se spalováním a pyrolýzou patří mezi procesy využívající vysoké teploty ke zpracování paliva a jeho přeměně na energeticky lépe využitelné produkty plynného charakteru. Běžně se jako zplyňovací médium používá vzduch, vodní pára nebo O_2 v podstechiometrickém množství. Alternativně lze použít také CO_2. Pro využití CO_2 jako zplyňovacího média je vhodné použít taveninu soli jako reakční médium mezi palivem a plynem. V rámci experimentálního procesu se optimalizace zplyňování odvíjí od nastavené teploty, objemu nadávkovaného odpadu a průtoku zplyňovacího média a reakční doby odpadu v reaktoru.

Metodika

V rámci experimentální činnosti bylo zkoumáno jedno-reaktorové uspořádání MSG s alkalickou taveninou tvořenou eutektickou směsí LiNaK. Byly testovány dvě různé experimentální teploty – 800 °C a 900 °C – a vždy bylo nadávkováno stejné množství oleje. Analýza spalin probíhala kontinuálně metodou FID pro analýzu zbytkových organických látek v odplynech a analyzátorem plynů s NDIR detekcí pro analýzu CO a CO_2 a paramagnetickou detekcí pro analýzu O_2.

Výsledky

Během počátečních experimentů s taveninou LiNaK byly zatím provedeny čtyři preliminární experimenty vhodné k dalším úpravám procesu. Obecně se obsah CO v odplynech pohyboval kolem 3 % s mírně klesající tendencí při teplotě 800 °C, zatímco při vyšší teplotě měl rostoucí tendenci a pohyboval se opět kolem 3 %, s maximální hodnotou 4,5 %. Během experimentů byla použita stejná tavenina, a proto bylo sledováno i její nasycení nespalitelnými látkami. Obsah zbytkových organických látek byl velmi vysoký pohyboval se kolem 25 000 ppm s mírně rostoucím trendem.

Závěr

Preliminární experimenty prokázaly nízkou reakční účinnost zplyňování oleje v procesu MSG při počátečním nastavení. Vysoký obsah zbytkových organických látek v odplynech svědčí o krátkém reakčním čase, který bude nutné optimalizovat pro budoucí experimenty. Pro další experimentální činnost se plánuje úprava parametrů procesu, například množství zplyňovacího média nebo rychlosti dávkování oleje.

Grantová podpora

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OPERATING CONDITIONS OF A MOBILE POWER SOURCE WITH A PEM FUEL CELL

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The PEM fuel cell is an established technology for the efficient conversion of the chemical energy of the fuel into electrical energy. Its main advantages such as high efficiency, flexibility, process simplicity, non-toxic reaction products and quiet operation. The reaction products are only water, heat and electricity. This allows the use of fuel cells also in areas sensitive to exhalations, such as confined spaces or close proximity to people. The mobile PEM fuel cell unit can also be used as a temporary power source for telecommunication transmitters during outages. All these applications require the design of a suitable mobile control system for the PEM fuel cell stack.

However, the operation of the fuel cell is affected by ambient conditions such as temperature, humidity and air purity. It is therefore important to know the effect of these conditions on the operation of the fuel cell.

In the laboratory fuel cell, the conditions of the effect of proximity temperature, gas humidity and the effect of excess hydrogen and air were tested.
Comparison of load curves and parameters evaluated from electrochemical impedance spectra at different voltages was used to monitor the effect of specific parameters on cell performance. This allowed to identify the operating modes where the beam performance is reduced. These protocols will then be adapted into the control algorithms of the portable PEM fuel cell unit.

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ION SELECTIVE MEMBRANES SWELING FORCES AND THEIR ADAPTATION IN AN ELECTROMEMBRANE SEPARATION UNIT

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Electrodialysis (ED) represents a matured and well-established desalination and general electromembrane separation technology with typical plate-and-frame configuration. In order to satisfy application demands, there is a trend for an increasing dimension and operating temperature of the industrial ED, capable of high performance and efficiency in view of process time and system volume. The scale-up simply based on increasing membrane active area or number of membranes, without appropriate modifications of entire unit design, often lead to accentuation of negative effects that are normally negligible on a small scale.
One of the critical issues in larger scale represents dimensional changes of the ED stack, mainly due to membranes swelling and changes in mechanical properties of the stack materials as a respond to variation of operating conditions (temperature, electric current, salt concentration). When a robust rigid frame is used for stack assembly, such stack expansion may lead to an increase of the internal expansion forces causing irreversible mechanical damage of the materials used (membranes, spacers). On the contrary, the stack shrinking (e.g. due to membrane drying and deswelling) negatively affects the tightness. Consequently, the performance, reliability and lifetime of the apparatuses can be significantly exacerbated. Therefore, an autonomous (passive or active) system of compression force control has to be employed, which at each moment spontaneously adapts to stack dimensions keeping compression/expansion force at an optimal value. However, prior to a development of such system a deeper

fundamental understanding of the stack behaviour is required. We are mainly interested at (a) a qualitative and quantitative respond of the stack internal forces upon variation of different operating parameters, (b) uniformity of distribution of internal expansion forces, (c) dynamics (characteristic times) and reversibility of the stack dimensional changes, (d) effect of different compression forces and stack compression-expansion cycles to longer-term operation of the stack and also (e) stack tightness.

In the present study different regimes are investigated: (a) a regime with constant compression force in the pneumatic cylinders, or (b) constant stack dimension (rigid compression frame) during the entire experiment. There were found up to 3 different characteristic times in the stack dynamic respond to temperature change.

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OSDA-FREE SYNTHESIS OF AL-RICH *BEA ZEOLITE: KINETIC CONTROL AND CONTROL OF AL DISTRIBUTION IN THE FRAMEWORK*

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Recently, it was suggested that beta zeolites can accommodate binuclear iron centers, which play a key role in O_2 splitting and CH_4 oxidation [1]. However, formation of binuclear Fe sites requires high framework Al content and specific type of Al arrangement on the beta framework. The OSDA-free synthesis of zeolites represents a way for the synthesis of beta zeolite with high framework Al content. Further, it offers significant environmental and economic benefits but presents challenges in phase stability and kinetic control. This study focuses on the OSDA-free synthesis of Al-rich *BEA zeolite, which initially forms as a metastable phase but gradually transforms into thermodynamically stable MOR zeolite, following Ostwald's rule of stages. The synthesis is a dynamic process where crystallization and dissolution occur simultaneously. Once MOR zeolite begins to form, it depletes Al and Si from the synthesis mixture, leading to the rapid dissolution of *BEA under hydrothermal conditions. The choice of Al and Si sources plays a crucial role not only in phase selectivity, with properly soluble precursors and stable *BEA seeds enabling kinetic control, allowing high yields of *BEA before MOR becomes dominant [2-4], but also represents a key for the control of distribution in the zeolite framework [5].

The developed template-free synthesis ensures a low-defect structure with a high fraction of Al-pairs, which in turn stabilize these binuclear iron centers, as it was experimentally confirmed by their ability to activate O_2, stabilize reactive oxygen species, and efficiently oxidize CH_4 [6].

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References

[1] Tabor, E.; Lemishka, M.; Olszowka, J.; Mlekodaj, K.; Dedecek, J.; Andrikopoulos, P.; Sklenak, S., ACS Catal. 2021, 11, 2340
[2] Sazama, P.; Mokrzycki, L.; Wichterlova, B.; Vondorva, A.; Pilar, R.; Dedecek, J.; Sklenak, S.; Tabor, E.,Journal of Catalysis 2015, 332, 201
[3] Sazama, P.; Tabor, E.; Klein, P.; Wichterlova, B.; Sklenak, S.; Mokrzycki, L.; Pashkova, V.; Ogura, M.; Dedecek, J., Journal of Catalysis 2016, 333, 102
[4] Pilar, R.; Moravkova, M.; Sadovska, G.; Sklenak, S.; Brabec, L.; Pastvova, J.; Sazama, P., Microporous Mesoporous Mater. 2022, 333, 111726
[5] Gabova, V.; Dedecek, J.; Cejka, J., Chem. Commun., 2003, 10, 1196
[6] Kornas, A.; Tabor, E.; Wierzbicki, D.; Olszowka, J.; Pilar, R.; Dedecek, J.; Sliwa, M.; Jirglova, H.; Sklenak, S.; Zbik, D.; Mlekodaj, K., Applied Catal. B: Enviromental 2023, 336, 122915

PCB - A LASTING ENVIRONMENTAL BURDEN IN SLOVAKIA?

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Introduction

Polychlorinated biphenyls (PCBs) are a group of organic compounds known for their high stability, toxicity, and resistance to degradation. They consist of 209 congeners, which differ in the number and position of chlorine atoms on the biphenyl rings, affecting their physicochemical properties. In the past, PCBs were widely used in industry due to their insulating properties, non-flammability, and chemical stability. However, they can infiltrate various ecosystems and persist for years without significant biodegradation or chemical transformation.

A wide range of commercial PCB-containing products have been manufactured under different trade names. Chemko Strážske produced PCB mixtures known as Delor 106 and Delor 103, which were primarily used as dielectric fluids in capacitors and transformers. The objective of this study was to evaluate the efficiency of decontaminating a working solution containing these contaminants.

Methodology

At the beginning of the experiment, a stock solution containing Delor 106 and Delor 103 was prepared and subsequently mixed with cyclohexane. After the phase interface stabilized, a sample was taken from the upper cyclohexane layer and analyzed using gas chromatography.

To assess the decontamination efficiency, carbon sorbents and humic acids were used. Several types of sorbents were tested by mixing them with the stock solution. After filtration, the treated solution was injected into a gas chromatograph, and the resulting chromatograms were compared.

Results

The analysis showed that the sorbent labeled SAMB exhibited the highest efficiency in removing PCB congeners. In contrast, the sorbent SABE was the least effective, showing the lowest selectivity and adsorption capacity.

Conclusion

This study focused on evaluating different types of carbon sorbents and humic acids for PCB decontamination. The results indicate that carbon sorbents are the most effective, as even a small amount (approximately 100 mg) was able to nearly eliminate all biphenyl congeners from the tested solution.

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INORGANIC TECHNOLOGY

POSTERS

MESOPORIZATION OF *BEA ZEOLITE BY HOT LIQUID WATER AND ITS MECHANISM

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Introduction

Zeolites were recently shown to be promising catalysts for biomass related transformations [1,2]. However, there are limitations connected with the transport of large(r) molecules in the microporous channel system of the zeolite. Although mesoporous zeolites were highly recently reported, *BEA zeolite with 3D channel system of twelve-member ring channels and USY zeolite with cavities interconnected by twelve member rings represent commercially available silica rich alumosilicate zeolite catalysts with largest pores. Nevertheless, this drawback can be overcome by the introduction of mesopores to the microporous zeolite crystal. However, the methods employed for the mesopores formations are usually not ecologically friendly.

Experimental

The efect of hot liquid water treatment onbeta zeolites was investigated. Commertial beta zeolites with Si/Al 12.5 – 18 were trweated under various temperatures in hot liquid water. Surface area and micro- and mezoporozity were evaluated using nitrogen adsoorption, crystalllinity of treated zeolites by powder x-ray diffraction, state of Al and Si atom by ^{29}Si and ^{27}Al MAS NMR spectroscopy.

Results

The employment of HWT at 95 °C led to increasing of mesopores in all studied beta zeolites. Mesopore formation starts by dealumination followed by desilication and finally by leaching of Al and Si from the channel system.

Conclusions

Hot liquid water treatment represents new, simple and ecologically friendly method for the introduction of mesopores to the beta zeolite catalysts.

Acknowledgement

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FUNCTIONAL PEROVSKITE-BASED COOL PIGMENTS: SYNTHESIS, CHARACTERIZATION, AND NIR REFLECTIVITY EVALUATION

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The energy demands associated with building operation represent not only an economic challenge but also a significant environmental concerns. According to estimates, approximately 50% of global electricity production is consumed for the thermal management of buildings, with heating in winter and cooling in summer [1]. However, this issue is not limited to buildings alone; it also affects vehicles and, in fact, the surfaces of virtually all objects exposed to sunlight.

A wide range of contemporary materials has been shown to reduce energy consumption. Some function as effective thermal insulators, including phase change materials, porous materials, and even repurposed industrial waste. Advanced surface coatings have demonstrated efficacy in protecting surfaces from mechanical damage and extreme temperatures. Additionally, specialized high-reflectivity coatings, the functional inorganic pigments known as "cooling pigments", have been identified as a potential solution to this challenge [2].

Inorganic pigments with a perovskite structure represent a highly promising class of functional materials capable of reflecting solar radiation, thereby reducing surface heating. Perovskite pigments are cost-effective, relatively easy to synthesize, and thus serve as ideal candidates for affordable yet efficient cooling pigments. In this study, $CaSn_{0.9}M_{0.1}O_3$ (M = Mn, Fe) and $SrSn_{0.9}Mn_{0.1}O_3$ pigments were synthesized using various routes, including solid-state reactions and precipitation techniques. Following calcination, the resulting products were characterized using X-ray diffraction (XRD) and UV-VIS-NIR spectroscopy. The particle size distribution of the powders was analysed via laser light scattering. The influence of elemental composition (Ca/Sr ions and Mn/Fe dopants) on NIR reflectivity and colour parameters was systematically evaluated.

[1] EIA, 2025. International Energy Outlook 2024. U.S. Energy Information Administration

[2] Hroch J., Dohnalová Ž., Šulcová P., Ceramics International, 2023, 49 (15), 25246–25252

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Optimization of the preparation of nucleation seeds intended for the production of rutile type TiO_2 and evaluation of their efficiency

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The optimization of nucleation seeds preparation to produce rutile-type titanium dioxide (TiO_2) is a critical step in enhancing the efficiency and cost-effectiveness of the manufacturing process. This study focuses on refining the methods used to prepare nucleation seeds, aiming to improve their effectiveness in promoting the formation of rutile TiO_2 by adjusting the ratio of reagents used in their preparation. Various evaluation techniques were used to assess prepared nucleation seeds. While the optimized preparation methods showed some improvement, the overall efficiency of the rutilization process did not exhibit significant enhancement. Despite this, the findings provide valuable insights into the preparation techniques and highlight areas for further research to achieve better efficiency and cost savings in the production of rutile TiO_2.

This research was conducted in collaboration with Precheza a.s.

THE ROLE OF DOUBLE SALTS AND X-RAY ANALYSIS IN QUALITY CONTROL OF ASN FERTILIZERS

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Ammonium nitrate (AN) and ammonium sulfate (AS) are widely known to form double salts: 3AN·AS ($3NH_4NO_3{\cdot}(NH_4)_2SO_4$) and 2AN·AS ($2NH_4NO_3{\cdot}(NH_4)_2SO_4$). These double salts enhance nutrient delivery efficiency compared to AN alone. Ammonium Sulfate Nitrate (ASN)-based fertilizers are designed to provide targeted nutrition and high yields by combining the prolonged availability of ammoniacal nitrogen (NH_4^+) with the rapid effect of nitrate nitrogen (NO_3^-), along with the multiple agricultural benefits of sulfur - a nutrient that has been increasingly deficient in many soils in recent years.
One of the major physical challenges encountered during the handling, transport, storage, and use of ASN fertilizers is agglomeration (caking) and dust formation. The

severity of quality deterioration can be influenced by several factors, including phase composition, moisture content, particle structure, mechanical strength, hygroscopic properties, product temperature, ambient conditions, storage duration and applied pressure. Studies have shown that the presence of mixed salts 3AN˙AS and 2AN˙AS significantly impacts fertilizer quality.

Given that X-ray Powder Diffraction (XRPD) analysis is widely used for quality control in industrial fertilizer production, a new X-ray method has been developed. This method is based on determining the ratio of the integral intensities of the diffraction lines corresponding to the 3AN˙AS and 2AN˙AS components. The ratio obtained through line profile analysis serves as an effective screening test for assessing fertilizer quality immediately after production. Based on this ratio, it is also possible to estimate product quality changes over long-term storage.

VISCOSITY AND CRYSTAL GROWTH KINETICS IN GESE$_2$ AMORPHOUS CHALCOGENIDE GLASS

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Chalcogenide glasses have unique physical properties, making them a point of interest in many fields of study in recent years. They are widely used in the optical and electrotechnical industry due to their high refraction index and infrared spectrum transmittance, where the perfectly stable amorphous phase is required. Crystallization is undesirable in optical applications, but it is helpful in preparing phase-change materials for data storage. In both cases, the knowledge of crystallization kinetics is, therefore, vital.

Crystals are formed when the structural units have enough mobility. Higher mobility of structural units can be observed at higher temperatures, specifically in an undercooled melt area, which is a temperature interval limited by the temperature of glass transformation and melting temperature. To fully understand the kinetic properties of GeSe$_2$ material, a series of viscosity and crystal growth rate measurements were performed.

The viscosity properties of amorphous samples were studied using two methods, one of which is the thermomechanical analysis (TMA), used for measuring the viscosity of bulk samples. The second method, which was nanoindentation (NI), was used mainly for measuring the viscosity of samples in the form of a thin film but was also used to verify the viscosity values of bulk samples measured by TMA. The obtained viscosity data were then described by the MYEGA viscosity model.

The amorphous glass was annealed either ex-situ, in a furnace, or in-situ in a computer-programmable heating stage. The growing crystals were observed under an infrared microscope and the crystal growth rate was calculated from the change of length in time. The dependency of crystal growth rate on temperature was described by a proper kinetic growth model, which extrapolates growth data in a broad range of temperatures.

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APPLIED CATALYSIS AND ORGANIC TECHNOLOGY

LECTURES

MOLYBDENUM SILICATE MICROSPHERES PREPARED VIA A COMBINED CONDENSATION APPROACH AND THEIR CATALYTIC ACTIVITY IN PROPYLENE METATHESIS

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Olefin metathesis is a versatile reaction involving the rearrangement of C=C bonds used in various applications, ranging from the synthesis of fine chemicals to the large-scale production of petroleum products. In this study, we present molybdenum silicate microspheres as heterogeneous catalysts for propylene metathesis. These microspheres are synthesized through a combined approach based on microwave-assisted heating followed by a condensation reaction. Microwave-assisted reaction involving bis(acetylacetonato)dioxomolybdenum(VI) and biphenyl-4,4′-dicarboxylic acid, forming a hybrid molybdenum biphenyl dicarboxylate precursor. This precursor is then mixed with (3-Aminopropyl)triethoxysilane and this condensation step produces hybrid molybdenum silicate solids. After their calcination at 500 °C in an air atmosphere, the resulting amorphous and porous Mo-SiO2 microspheres containing highly dispersed molybdate species are obtained.[1,2] The physical properties of these microspheres were analyzed using electron microscopy, and nitrogen adsorption isotherms, X-ray photoelectron spectroscopy, ^{29}Si solid-state NMR. In-situ ultraviolet-visible diffuse reflectance spectroscopy and time-of-flight secondary ion mass spectrometry revealed that these catalysts have homogeneously dispersed MoO_x species, which exhibit high catalytic activity in heterogeneous propylene metathesis. Compared to traditional silica-supported MoO_x catalysts prepared by the incipient wetness impregnation method, the Mo-SiO2 microspheres demonstrated nearly two orders of magnitude higher steady-state propylene metathesis rates, reaching values as high as 4.11 × 10–5 mol g^{-1} s^{-1}.

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References:

(1) Skoda, D.; Hanulikova, B.; Styskalik, A.; Vykoukal, V.; Machac, P.; Urbanek, P.; Domincova Bergerova, E.; Simonikova, L.; Kuritka, I. J. Ind. Eng. Chem. 2022, 107, 320–332. https://doi.org/10.1016/j.jiec.2021.12.001.

(2) Skoda, D.; Zhu, R.; Hanulikova, B.; Styskalik, A.; Vykoukal, V.; Machac, P.; Simonikova, L.; Kuritka, I.; Poleunis, C.; Debecker, D. P.; et al. ACS Catal. 2023, 13 (19), 12970–12982. https://doi.org/10.1021/acscatal.3c02045.

CATALYST MANAGEMENT AT ORLEN UNIPETROL - STUDY OF PROCESS CONDITIONS USED FOR STABILIZATION OF SPENT CATALYST

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Introduction

At ORLEN Unipetrol, catalysts play a key role. Efficient catalyst management is the key to savings and sustainability. Catalysts save energy and money, help protect the environment, increase the efficiency of the production process, etc. The company therefore devotes considerable effort to this area.

One of ORLEN Unipetrol's key products is benzene. Benzene is produced by hydrodealkylation at the Pyrotol unit. It is a thermocatalytic process for the treatment of the aromatic C_9 fraction using Cr_2O_3/Al_2O_3. Chromium-containing catalysts have been intensively monitored, especially recently, for the presence of Cr^{6+}. Oxidation of the chromium catalyst can occur mainly during reactor shutdown. By optimising the Cr^{3+} stabilisation process during reactor shutdown, the Cr^{6+} concentration can be reduced below the legally permitted levels, which opens up further opportunities for recycling spent catalyst and meeting ORLEN Unipetrol RPA's objectives correlated with EU targets on metal recycling and resource efficiency.

Methodology

The aim of the work was to study the conditions of the Cr^{3+} stabilization process to avoid their oxidation to Cr^{6+} during reactor shutdown. The unloaded spent catalyst was characterized by temperature-programmed techniques (TPO, TPR), which allow to determine the reduction temperature and to describe the reduction process. The optimization of the stabilization process was carried out in a tubular lab continual flow reactor, where activities were mainly focused on effects related to H_2 partial pressure, reduction temperature and reduction time.

Results

A series of different conditions of the Cr^{3+} stabilization process were tested. It was found that Cr^{6+} could be effectively reduced by 80-90% and reclassification of spent catalyst could be possible.

Conclusion

The applicability of the Pyrotol catalyst stabilization process was assessed under realistic conditions and a balance sheet was prepared comparing the cost of catalyst stabilization versus the cost of disposal of the catalyst as hazardous waste.

ZEOLITE-CATALYSED GAS-PHASE SYNTHESIS OF AN ALTERNATIVE FUEL ADDITIVE

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The method for synthesis of unsymmetric ethers from a mixture of alcohols that our research team developed previously can be widely applied for other compounds[1,2]. Ethyl tetrahydrofurfuryl ether (ETFE) is a promising diesel fuel additive. Its cetane number is 80-90. The engine tests for various mixtures of conventional diesel fuel and ETFE showed positive results with regular engine operation, lower content of particulate matter, and sulphur[3]. Hereby, we applied the method for unsymmetric ether preparation on a mixture of bio-based tetrahydrofurfuryl alcohol (THFA)[4] and ethanol (EtOH).

We carried out reactions with a series of commercially available zeolites. Catalytic tests were carried out in a fixed-bed flow reactor filled with 2 g of pressed and sieved H-form zeolite in the presence of inert nitrogen. In a model experiment, a mixture of EtOH and THFA in mass ratio of 5:1 was fed into the reactor at weight hourly space velocity (WHSV) of 0.25 $g_{THFA} \cdot g_{cat}^{-1} \cdot h^{-1}$. The reaction was performed at 140 °C. Hourly samples of reaction mixture were analyzed by gas chromatography.

The results of preliminary tests with various zeolite structures show, that highest ETFE yield, and selectivity achieved in the presence of H-ZSM-5. Hence, we carried out the examination of technical conditions and catalyst properties with this structure type. At optimized reaction conditions, we achieved selectivity of ETFE formation of 27.8 % at THFA conversion of 50.3 %.

Gas-phase synthesis of ETFE is a promising method for the preparation of an alternative diesel fuel additive due to its mild reaction conditions and utilization of bio-based feedstock. Quick deactivation of the catalyst is an important topic for further research.

Financial support

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References

1 Soták, T.; Magyarová, Z.; Shamzhy, M.; Kubů, M.; Gołąbek, K.; Čejka, J.; Hronec, M. Applied Catalysis A: General 2021, 618, 118122.

2 Silná, Z.; Lopatka, P.; Soták, T. 2nd Forum of Young Researchers on Heterogeneous Catalysis, BOOK OF ABSTRACTS. Hungarian Catalysis Society of the HAS, Szeged, 2024. ISBN 978-963-7351-36-5.
3 de Jong, E.; Vijlbrief, T.; Hijkoop, R.; Gruter, G.-J. M.; van den Waal, J. C. Biomass and Bioenergy 2012, 36, 151-159.
4 Lan, J.; Liu, P.; Fu, P.; Liu, X.; Xie, M.; Jiang, S.; Wen, H.; Zhou, Y.; Wang, J. Microporous and Mesoporous Materials 2021, 322, 111161.

EXPLORING 3D MICROSTRUCTURAL CHANGES IN WORKING PT-CO CATALYSTS OF A FUEL CELL VIA ELECTRON TOMOGRAPHY

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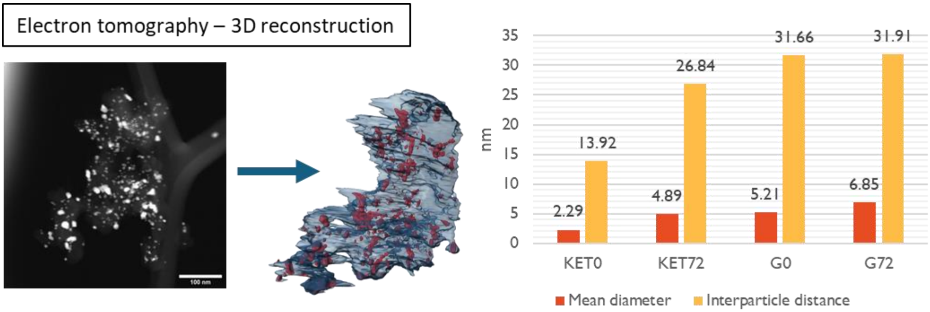
Transmission electron microscopy (TEM) provides crucial insights into catalysts at near-atomic resolution. However, conventional TEM provides only 2D projections of inherently 3D structures, limiting the spatial understanding of catalyst morphology. To overcome this limitation, electron tomography is used to reconstruct 3D information. In this study, we utilized electron tomography to examine the spatial and size distribution of metal active sites in High Temperature-Proton Exchange Membrane Fuel Cell (HT-PEMFC) Pt/Co catalysts. Spacial information is crucial in understanding of the rapid degradation of Pt/Co nanocatalysts which leads to a significant reduction in fuel cell lifetime. Two novel types of catalyst were synthesized: one Pt/Co supported on graphene oxide (G) and the other Pt/Co on carbon Ketjen Black (KET). These catalysts were tested under standard operating conditions (180 °C, acidic environment). Electron tomography images were captured before and after the workload. Both bright-field and dark-field images were segmented to create 3D models at nanoscale resolution. Based on the segmented 3D model, we identify an average increase of metal particles by 113 % and 31 % during the 72 hours. The average distance between the individual metal nanoparticles increased by 92 % and 1%. These quantities suggest the degradation mechanism of metal nanoparticles by Ostwald ripening or coalescence. These changes, undetectable by conventional 2D TEM, highlight the necessity of 3D electron tomography for evaluating electrocatalyst stability under standard conditions.



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OXIDATIVE MODIFICATION OF CELLULOSE

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Introduction

Cellulose is the most abundant natural polymer and a valuable starting material for a wide range of applications. One of the key chemical modifications of cellulose is oxidation, which produces biocompatible and bioresorbable polymers. These materials are utilized in medical and pharmaceutical applications, including haemostatic agents, anti-adhesion barriers, tablet formulation, pharmaceutical gels, and tissue engineering. Furthermore, oxidized cellulose serves as a precursor for nanocellulose production and, upon deep oxidation, can be converted into formic and acetic acid.

Methodology

Selective oxidation primarily converts the primary hydroxyl groups of anhydroglucose units into carboxyl groups. The process is highly dependent on reaction conditions such as the choice of oxidizing agent, pH, temperature, and solvent system. The oxidation typically yields aldehyde or carboxyl functionalities at primary hydroxyl groups, whereas secondary hydroxyls may transform into ketone or aldehyde groups, occasionally leading to glucose ring cleavage. One of the most effective oxidation methods involves nitroxyl radicals, particularly the TEMPO (2,2,6,6-tetramethylpiperidine-N-oxyl) system.

Results

TEMPO-assisted oxidation employs nitrosonium cations, generated in situ by the reaction of TEMPO with an oxidizing agent, such as sodium hypochlorite, under alkaline conditions (pH = 10.5). This process achieves high selectivity and conversion efficiency, yielding oxidized cellulose with a carboxyl content of approximately 0.7–0.9 mmol COOH/g. To enhance the degree of oxidation, a post-treatment with sodium chlorite (NaClO2) can be applied, increasing the carboxyl content to 1.0–1.15 mmol COOH/g.

Conclusion

In our study, a one-step TEMPO-assisted oxidation process was developed and validated on a pilot scale. This method consistently produced oxidized cellulose with a carboxyl content exceeding 1.0 mmol COOH/g. The key process steps include preparation of the oxidizing agent, cellulose treatment, oxidation, and final product purification. The presentation will detail the technological aspects of this process.

Acknowledgement
This research was supported by the Slovak grant APVV-19-0479.

HIGH ENTROPY TRANSITION METAL PHOSHIDES FOR ALKALINE WATER SPLITTING: BALANCING COMPOSITION AND ACTIVITY

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Hydrogen's high energy density and versatility make it key to decarbonizing industry, transport, and energy storage. While water splitting is a promising production method, it requires significant energy. Current platinum catalysts are highly effective but expensive and scarce. Therefore, cost-effective, abundant, and scalable alternatives with comparable activity and stability are needed. High-entropy phosphides (HEP), composed of five or more elements, offer a promising solution. Their complex structure promotes synergistic interactions, optimizes electronic structures, and increases active sites, leading to efficient and stable catalysis.

This study explores the incorporation of transition metals into a molybdenum phosphide framewrok to develop a high-entropy transition metal phosphide catalyst. A simple sol-gel synthesis was used to progressively add nickel, copper, and manganese to a binary MoFeP, creating a series of catalysts with increasing compositional complexity.

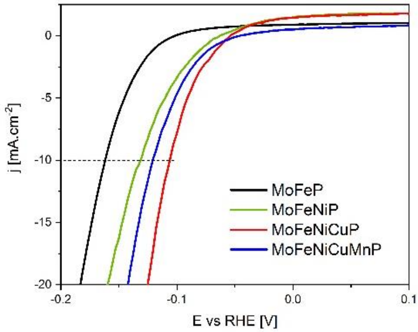

Figure 1 Linear sweep voltammetry curves for prepared catalysts measured in 1 M KOH

Electrocatalytic activity was evaluated in 1 M KOH using linear sweep voltammetry (Fig. 1). Surprisingly, the five-metal high-entropy phosphide did not exhibit the highest activity. Instead, the four-metal phosphide achieved the best performance, requiring an overpotential of only 106 mV at 10 mA cm^{-2}, suggesting an optimal synergistic effect. The HEP, in contrast, required 121 mV to reach the same current density, possibly due to reduced active site accessibility with the addition of the fifth metal.

This study demonstrates that while increasing compositional complexity in transition

This work demonstrates that while increasing compositional complexity can improve the catalytic performance of transition metal phosphides, there's an optimal balance. These results offer valuable insights for designing multi-metallic catalysts, highlighting the importance of elemental synergy over the sheer number of incorporated metals.

Acknowledgements

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DESIGN OF TRANSITION METAL PHOSPHIDES AS ELECTROCATALYSTS FOR WATER SPLITTING.

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Environmental and socioeconomic concerns over fossil fuel use highlight the need for alternative energy sources. Hydrogen, with no carbon emissions, is seen as a key alternative fuel for a renewable energy economy. Water electrolysis offers a promising method for producing pure H2, but achieving an efficient and economical hydrogen evolution reaction (HER) rate is crucial for practical applications, balancing low overpotential and high efficiency.

Electrocatalysts improve HER rates, making the process more beneficial. Ideal materials should have good conductivity, high corrosion resistance, large surface area and be cost-effective. Noble metals, like platinum, have high catalytic activity but are limited by their high cost and scarcity for large-scale use.

Transition metals phosphides are the most used cathode material for water electrolysis due to their affordability and corrosion resistance. Their catalytic activity rises with d-electron filling of metal, peaking near full occupancy. However, HER also depends on adsorption, which strengthens as d-electron filling decreases. Enhancing electroactivity involves creating vacancies to improve hydrogen adsorption through electron pair formation. DFT (density functional theory) calculations are a useful tool for predicting the number of active sites and the effective mechanism for HER. Another approach is combining semi filled d orbital metals (e.g., Mo) with paired-electron metals (Fe, Co, Ni) for high synergism and excellent HER catalytic activity. The incorporation of phosphorus atoms introduces new ionic bonds (Niδ+– Pδ-), which not only weakens the typically strong Ni-H interactions, facilitating easier desorption and release of hydrogen, but also enhances stability and resistance.

Elemental doping, including multi-element co-doping, enables the modulation of materials at the lattice level, enhancing both electrocatalytic activity, and stability and will be a key direction employing new strategies to regulate the microstructure for future development of new family of electrocatalysis for water splitting.

Acknowledgement

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APPLIED CATALYSIS AND ORGANIC TECHNOLOGY

POSTERS

CARBON-BASED CATALYSTS IN THE OXIDATION OF CYCLOPENTANONE BY MOLECULAR OXYGEN

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Glutaric acid, which started to be an important chemical for the production of bioplastics, particularly surfactants, additives and biologically active substances, was in the past produced as a side product in the production of adipic acid. Other possibility is the oxidation of cyclopentanone and cyclopentanol by nitric acid, or the carbonylation of butyrolactone[1]. An alternative is the oxidation of cyclopentanone using oxygen or air. Recently, bio-furfural was shown as one of the most promissing platform molecule in the production of cyclopentanone[2]. In this work, the catalytic performance of metal loaded and metal-free carbon catalysts in the oxidation of cyclopentanone by molecular oxygen in solvent-free conditions was studied. Carbon black Vulcan was demineralized with hydrochloric acid, thermally treated in nitrogen atmosphere and modified with urea by impregnation method described in paper[3]. Carbon supported metal catalysts were prepared by wet impregnation method reported by Zou[4]. Samples were characterized by particle size distribution, XRPD, SEM, N_2-adsorption-desorption isotherms, X-ray microprobe analysis (EDX), XPS, acid-base titration, FTIR and Raman techniques. The catalytic tests were carried out in a thermostatic stirred glass reactor at 90 °C and 0.45 MPa. The reaction mixture was analysed by gas chromatography and GC-MS.

Metal-free catalysts performed comparably to Cu-loaded ones, however, we assume the possibility of a different reaction mechanism. Demineralization decreased slightly the surface pH and increased the number of surface acidic groups. In urea-modified catalyst treated at 500 °C the increase in the number of basic groups was evident. The applied treatments did not alter significantly the porosity and the crystallinity. The conversion of cyclopentanone and selectivities to glutaric acid and succinic acid depended on surface modification of carbon black Vulcan. The advantage of non-metal catalysts is their trouble-free recycling. The challenge remains, however, the recycling of unreacted cyclopentanone and the utilization of by-products.

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References

[1] R.W. Johnson, C.M. Pollock, R.R. Cantrell, Dicarboxylic acids. In: Kirk-Othmer Encyclopedia of Chemical Technology (2010).

[2] M. Hronec, K. Fulajtárová, I. Vávra, T. Soták, E. Dobročka, M. Mičušík, Appl. Catal. B Environ. 181, 210 (2016).

[3] M. Seredych, D. Hulicova-Jurcakova, G.Q. Lu, T.J. Bandosz, Carbon 46(11), 1475 (2008).

[4] G. Zou, W. Zhong, Q. Xu, J. Xiao, C. Liu., Y. Li, L. Mao, D. Yin, Catal. Commun. 58, 46 (2015).

TOPOCHEMICALLY SYNTHESIZED SI AND GE QUANTUM DOTS FOR INVESTIGATING POROUS NETWORKS IN SOLID CATALYSTS

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Si and Ge Quantum Dots (QDs) have become attractive materials for various applications, such as photodetectors, solar cells, drug delivery systems, or imaging or light-emitting diodes which could be used to explore accessible porous systems of solid materials. Due to their tunable optical and electronic properties, the relative non-toxicity, and the availability of starting materials, Si and Ge QDs represent sustainable alternatives to traditional quantum dots like those containing lead, particularly for large-scale production and environment-friendly, cost-effective applications. In this study, Si and Ge QDs were synthesized by topochemical deintercalation of Zintl phases $CaSi_2$ and $CaGe_2$, followed by Pt-catalysed solvothermal functionalisation with 1-alkynes. Fluorescence activity of the as-prepared QDs was measured using a fluorescence spectrometer and impacts of reaction conditions on sizes and shapes were examined with scanning transmission electron microscopy (STEM). Presented method produced generally polydisperse colloidal solutions of Si QDs with dominant population ~ 3 nm in diameters, exhibiting narrow excitation and emission spectra with maxima around 440 nm and 525 nm, respectively. Colloidal solutions of Ge QDs with dominant population ~ 2 nm in diameter, exhibiting narrow excitation and emission spectra with maxima around 380 nm and 480 nm, respectively. Polydisperse QDs were then separated through column chromatography to acquire isolated fractions, which were used in the study of the local pore accessibility of γ-Al_2O_3 extrudates – an industrially often used support of metal catalysts. Individual QDs stained catalyst particles were then investigated on confocal fluorescence microscopy to visualise the accessibility and interconnectivity of pore space. Z-stacking of individual focal planes allowed 3D reconstruction of the porous system, distinguishing pore volumes accessed by QDs differing in characteristic size. These findings present a new method for producing environmentally friendly and stable QDs derived from Si and Ge while demonstrating their potential for mapping porous systems of heterogeneous catalysts.

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

KATALYTICKÁ HYDROGENOLÝZA GLYCEROLU: PŘÍPRAVA BIO-1,2-PROPANDIOLU

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Úvod

Glycerol je vedlejší produkt vznikající při výrobě biopaliv a jeho efektivní valorizace je klíčová pro udržitelnou chemickou průmyslovou produkci. Jednou z možných cest jeho využití je katalytická hydrogenolýza, při které vzniká celá řada produktů, které se široce uplatňují v polymerní chemii a jiných průmyslových aplikacích. Cílem tohoto výzkumu je studium katalytické hydrogenolýzy glycerolu a porovnání použitých měděných katalyzátorů z hlediska konverze glycerolu a selektivity na jednotlivé produkty.

Metodika

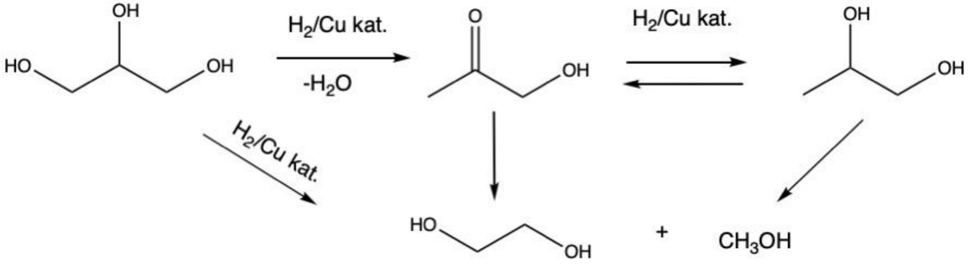
Experimenty byly provedeny v laboratorním trubkovém reaktoru s fixním ložem katalyzátoru za atmosférického tlaku. Testovány byly komerční hydrogenační katalyzátory, ale i katalyzátor připravený v laboratoři VŠCHT. Charakterizace katalyzátorů byla provedena pomocí BET analýzy povrchu, rentgenové difrakce (XRD) a programované desorpce (TPD). Kvantitativní analýza reakčních produktů byla provedena pomocí plynové chromatografie (GC). Optimalizace průmyslově relevantních podmínek byla modelována v softwaru Aspen Plus.

Výsledky

Bylo zjištěno, že měděné katalyzátory jsou pro hydrogenolýzu glycerolu aktivní až nad teplotou 220 °C. Dále bylo zjištěno, že reakce probíhá přes meziprodukt hydroxyaceton, který vzniká eliminací vody z gylcerolu. Hydroxyaceton je následně hydrogenován na požadovaný 1,2-propandiol. Kromě těchto látek byl nalezen ethylengylkol a methanol, jako produkty nežádoucí hydrogenolýzy C-C vazby.

Závěr

Získané výsledky poskytují základní přehled o průběhu hydrogenolýzy glycerolu a o složení reační směsi. Tyto výsledky budou dále použity pro technicko-ekonomickou studii výroby 1,2-propandiolu z glycerolu jako konkurenční zelený postup k zavedeným technologiím, které využívají fosilní zdroje.



MOO_3 AND ZNO MODIFIED MCM-41 - EFFECTIVE CATALYST IN NOPOL SYNTHESIS

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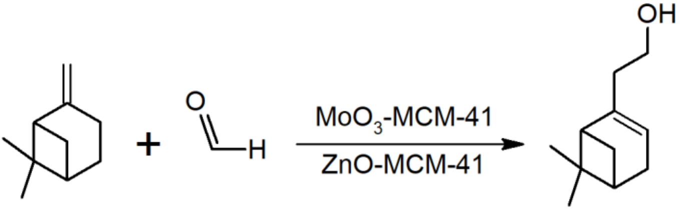
Nopol (2-(6,6-dimethyl-2-bicyclo[3.1.1]hept-2-enyl)ethanol) is bicyclic monoterpenic primary alcohol, which is used in agrochemical, food and perfumery industry. It is used to e.g. synthesize dithiphospahte pesticides, or as a fragrance . Nopol is usually synhesized by reaction of β-pinene (usually obtained from turpentine oil) with paraformaldehyde (Fig. 1) catalyzed by Lewis acid homogeneous catalyst (e.g. $ZnCl_2$).

Figure 1. Prins reaction of β-pinene with paraformaldehyde providing nopol



In this work we report utilization of MoO_3 and ZnO modified MCM-41 as effective heterogeneous catalysts in Prins reaction of β-pinene with paraformaldehyde providing nopol with high selectivity at high conversions. Materials modified by MoO_3 and ZnO (2 – 10 wt.%) were prepared by wet impregnation method followed by calcination. Prepared materials were characterized using X-ray fluorescence and nitrogen physisorption. Catalytic activity was tested using different solvents (benzonitrile, acetonitrile, toluene), temperature (60 – 120°C) and reactant molar ratio (1:1 – 1:3). Among MoO_3 modified MCM-41 the best result (90% conversion, 98% selectivity, 24 h) was obtained using molar ratio of reactants 1:2, 80°C, benzonitrile and 20 wt.% of 5wt.%MoO_3-MCM catalyst. Among ZnO modified MCM-41 the best result (96% conversion, 98% selectivity, 24 h) was obtained using molar ratio of reactants 1:2, 80°C, toluene and 20 wt.% of 5wt.%ZnO-MCM catalyst.

POLYMERS, COMPOSITES

LECTURES

NATURAL-BASED ANTIOXIDANTS FOR NATURAL RUBBER MIXTURES

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Rubbers are very important materials in the industry, used to produce tires, hoses, sealing elements, etc. They stand out in the ability to withstand significant deformation without damage, with this deformation being mostly reversible. One of the most important representatives is natural rubber. It has excellent tack for fabrication, and its vulcanizates have high tensile strength.

Vulcanized rubber, during long-term storage, slowly changes its properties; this process is called ageing. Usually, this is caused by chemical reactions with oxygen or ozone from the atmosphere. The weakest places in rubber to undergo these reactions are double bonds. To prevent degradation, rubber should be stabilized with antidegradants. Antioxidants protect rubber from the impact of oxygen, whereas antiozonants protect it from reacting with ozone. Antioxidants can be divided into two major groups based on their mechanism of action: those that interrupt the kinetic chain and hydroperoxide deactivators.

In this work different natural antioxidants were used, like:

2-isopropyl-5-methylphenol (Thymol), 5-isopropyl-2-methylphenol (Carvacrol), DL- α-tocopherol, Cashew nut shell liquid (CNSL), Green tea extract and trans-β-farnesene. The chosen antioxidants will then be compared with two antidegradant systems: pure 1,2-dihydro-2,2,4-trimethylquinoline (TMQ) and a typical commercial system containing TMQ + 6PPD.

This work focused on comparing mixtures of natural rubber with various natural antioxidants with mixtures with synthetic antioxidants. Artificial ageing tests were performed and the degradation of the vulcanizates was evaluated and mechanical properties were compared.

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NATURAL RUBBER VULCANIZATION ACTIVATED BY ZINC OXIDE FIBRES

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Natural rubber is one of the most widely used materials in the rubber industry. Its main reaction is called vulcanisation. The vulcanisation reaction can be accelerated by using special chemical compounds called activators. Activators lower the activation energy of vulcanisation and make the reaction more effective. The most commonly used activator for sulphur vulcanisation of natural rubber is zinc oxide. It has great activation ability at relatively low cost. Its main disadvantage is its potential toxicity to aquatic organisms at certain concentrations. A major problem is the release of zinc oxide into the environment during the production, processing and use of the products (e.g. tyres). In this work, the a special type of zinc oxide in form of fibers as an activator was tested against commonly used and commercialy available types of zinc oxide. Cured rubbers activated with a special type of zinc oxide showed better mechanical properties than those activated with normal zinc oxides. Thus,the amount of zinc oxide in rubber can be reduced while maintaining the same mechanical properties. Rubber vulcanisation kinetics and cross-link density of cured rubbers were investigated. Mechanical properties such as tensile strength, tear resistance and hardness were also evaluated.

MODIFICATION OF THE PROPERTIES OF NITRILE RUBBER BLENDS WITH THERMOPLASTIC STARCH AND SILANES

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Úvod

In recent years, the trend in the rubber industry has been the use of renewable resources in rubber compounds. Thermoplastic starch appears to be a promising material as an additive to rubber compounds. For this purpose, nitrile rubber (NBR) was used, into which thermoplastic potato starch (TPS) was mixed. Mixtures were prepared in various weight ratios of NBR:TPS, and a group of mixtures was also prepared, which were additionally enriched with the coupling agents silane Si69 and Si264. Among the evaluated properties of the materials, the most interesting results were the oil absorption rates in hydraulic oil. NBR is classified among the significant oil-resistant rubbers, and thus this property is essential for its industrial use, such as in the production of seals for the transportation of oil-based products. It was very positive to find out that NBR rubbers containing TPS showed lower oil absorption in hydraulic oil than pure NBR rubbers. Moreover, materials enriched with the Si69 showed even lower oil absorption than the previously mentioned mixtures, which represents great potential.

IN SITU FORMED POLY(ε-CAPROLACTONE) AS A NON-TOXIC PLASTICIZER OF POLY(VINYL CHLORIDE)

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Poly(vinyl chloride) (PVC) is one of the most widely spread synthetic polymer in the world, because of its cheap production and chemical resistance. It is produced in two basic types: the hard PVC (without plasticizers), and soft (with plasticizers). It is irreplaceable in many applications including medical ones. The production of soft PVC concerns a great issue with low-molar weight plasticizers that are volatile and can migrate from the polymer, some of them being harmful to human health. Therefore, low-molar weight plasticizers are often replaced with polymeric ones, which are, however, less effective and require higher processing temperature. Therefore, we have studied a specific method of PVC plasticization consisting in the mixing of PVC melt with monomeric ε-caprolactone. During the mixing, *in situ* polymerization of the ε-caprolactone occurs, resulting in the formation of poly(ε-caprolactone), a non-toxic and bio-degradable polymeric plasticizer. Here, the thermal stabilizer of PVC, e.g., zinc 2-ethylhexanoate, plays at the same time a role of initiator of ε-caprolactone polymerization. Such way, we obtain plasticized PVC, the thermal stability, softening range and mechanical properties of which are comparable with the ones of conventional plasticizers.

CHARACTERIZATION OF ELASTOMER DURABILITY: INSIGHT INTO COMPRESSION SET AND STRESS RELAXATION

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Elastomers are crucial materials used in a wide range of applications, from erasers, shoe soles, hoses, and seals to more complex products like tires and conveyor belts. Each product must meet the specific properties required in its field. For example, hoses must withstand the pressure and chemical nature of the fluid being conveyed, while tires must endure internal pressure, the load from the car's weight, and the effects of surface roughness. Products such as gaskets, anti-vibration pads, and silent blocks must withstand permanent loads. This permanent deformation, along with the effects of temperature and environmental factors, significantly affects the lifespan of these products.

To characterize the durability of rubber materials under permanent compression or tension, two main methods can be used: compression (or tension) set and stress relaxation. The compression (or tension) set describes the elastic recovery behaviour after specific deformation over various times and temperatures. The measurement of stress relaxation appears similar; however, in this case, the time-dependence of stress under a constant strain is observed. This polymer behaviour is measured when a fixed deformation is applied to the specimen, and the load required for further compression as a function of time is recorded.

Our research focuses on the characterization of compression set and, particularly, stress relaxation. Our research group is involved in developing a modified device for stress relaxation measurement. This device consists of a main part used for measurement the force necessary for sample deformation and contains several cells where samples can be exposed to elevated temperatures or chemicals. More detailed information will be provided in the presentation.

RECYCLING AND UPGRADING OF PLASTIC WASTE BY SOLVENT BASED METHODS

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Polyethylene (PE) and polypropylene (PP) dominate plastic and waste production as they constitute half of the world's production of synthetic polymers but also half of the world's plastic waste. Despite PE and PP share in plastic waste, we can mark PE and PP as environmentally friendly materials considering their chemical composition. However, they are full of additives containing problematic elements for recycling (e.g., nitrogen, oxygen, sulfur, chlorine, fluorine). The additive removal process can be stressful to polymer materials and polymer chains can degrade. For final processing we are developing a fractionation method to remove degraded fraction and rise the value of the processed polymer. Fractionation method is also an option to separate multilayer or composite textile materials, e.g., COT/PES or COT/PA.

Small lab-scale apparatuses were constructed for polymer purification and fractionation at various experimental conditions. The experience from these small units was employed in the scaled-up units capable to process pilot-scale batches. Obtaining larger quantities of recycled plastic materials now unlocks possibilities of their thorough characterization (e.g., melt flow ratio, MFR) and testing in applications.

Additives removal experiments were conducted with real plastic waste to proof that decolorizing and removal of other additives is possible. The systematic engineering design of additives removal required the preparation of the calibration sets of polymer granules with well-defined content of colorants and/or additives.

The solvent system selection is crucial for both additives removal and fractionation, and the problem is to choose the best one with respect to performance, toxicity and solvent recovery. There is no chance to experimentally try every known solvent. Instead, we first employed a simple theoretical description using Hansen solubility parameters. But this simple method failed to describe the polymer-solvent-additive system correctly due to the empirical foundation of this method. Therefore we moved to COSMO-SAC method

calculating the quantum-mechanical properties and interactions of solvents, polymers and additives, and the simulation results were validated experimentally.
The textiles recycling experiments (with mixed fibers composition) were conducted with a set of selected solvents and several promising approaches were identified. The separated and decolorized textile samples were systematically inspected also by digital microscopy.

COUPLED THERMOGRAVIMETRIC TECHNIQUES FOR ADVANCED POLYMER ANALYSES

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Nowadays, thermogravimetric analysis (TGA) is a widely available technique that can be used to study stability and degradation behaviour of various materials, including polymers by measuring weight loss at a given temperature/time. However, it has its limitation while used on its own; therefore, coupling to other analytical intruments, such as infrared spectroscope (FTIR), mass spectrometer (MS), or potentiometric titration (PT) [1] is necesarry to further describe the released decomposition, or degradation products.
In our work, TGA coupled with MS or PT were used to describe decomposition products, and quantify hydrogen chloride released from halogenated polymers.
Data from MS measurements allowed the separation of the degradation of the polymer itself from that of other components in the material. PT measurement quantified hydrogen chloride released during dynamic thermogravimetric measurements.
The data obtained will contribute significantly to the description of the degradation of studied materials, including additives, and can be used in the future to study degradation kinetics.

This work was supported from the grant of Specific university research – grant No A1_FCHT_2025_001 and grant No A2_FCHT_2025_023.

[1] Uřičář, J.; Chodounská, A.; Benešová, V.; Brožek, J.; Kalousková, R.; Coupled Thermogravimetric Analysis-Potentiometric Titration for Complex Analysis of Poly(vinyl chloride) Thermal Stability; ACS Measurement Science, 2025, 5, 1, 70–73, https://doi.org/10.1021/acsmeasuresciau.4c00090

SEPARATION OF RACEMIC MIXTURES USING CHIRAL NON-POROUS MEMBRANES

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Nafion117® membranes were modified using three different cationic cyclodextrin (CD) derivatives through strong ionic bonding. These CD derivatives featured a bis(methylimidazolium) (MIM2) cationic anchor covalently attached to the CD unit, either directly or via diethylene glycol (DEG) or tetraethylene glycol (TEEG) spacers. The modified membranes were evaluated for their enantioselective separation capabilities using a model racemic mixture of D/L-tryptophan in water. Various experimental setups—pertraction, two types of sorption, and pressure-driven membrane separation—were employed to characterize the membranes and assess their efficiency in enantiomeric separation. The highest enantiomeric excess values were achieved with CD-MIM2 and CD-DEG-MIM2 membranes, reaching 14% and 44%, respectively, over 280 days. The CD-TEEG-MIM2 membrane, which initially exhibited the lowest separation performance due to its longer spacer, showed a significant improvement when subjected to pertraction, increasing its enantiomeric excess from 2% to 27% within 80 days. While sorption played a crucial role in pertraction, the process notably enhanced the overall separation of the racemic mixture. The pressure-driven method, on the other hand, enabled a continuous and more rapid operation (see Fig. 1), demonstrating the potential for large-scale, continuous production of enantiopure compounds. This advancement could open new opportunities for commercial applications, addressing the high demand for efficient chiral separation techniques. A detailed comparison with previously published chiral membranes [2,3] will be discussed at the conclusion of the lecture.

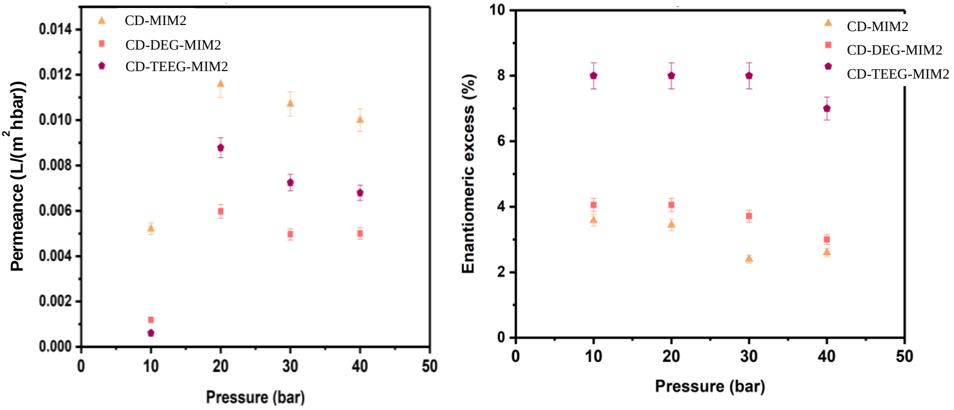

Figure 1: Evolution of the permeance of tryptophan solution accross CD modified membranes and the enantiomeric excess of D-Trp over L-Trp in a pressure driven separation set-up.

Acknowledgments
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References

[1] Izák, P. et al., *Separation and Purification Technology* **2021**, *266*, 118538.
[2] Brozova, L, et al., Langmuir, **2020**, 36 (42), 12723-12734.
[3] Izák, P. et al., Journal of Membrane Science, **2020**, 596, 117728.

DEVELOPMENT OF SUSTAINABLE MATERIALS BASED ON STARCH WITH NATURAL FILLERS

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Plastics nowadays are pervasive in almost all spheres of our lives. Production of them is 99 % based on fossil fuels. Unfortunately, that resource is known to be non-renewable, besides that weak point conventional plastics have another critical disadvantage as slow-moving decomposition for hundreds of years. This causes irreversible damage to the ecosystem, because of pollution all around the world. Thus, to reduce the negative influence on the environment, we have proposed the development of material based on starch, which is completely biodegradable and it is one of the most abundant polysaccharide on the planet. In this research, the structural characteristics of starch and its behavior after addition of biodegradable fillers will be discussed. Through further processing, raw starch will be transformed into thermoplastic starch (TPS)**.** During the material development procedure considering adding the following biodegradable fillers (BF), sourced from different spheres of industry which are popular not only in Czech Republic but also all around the world. The fillers used are sugar beet pulp, grape pomace, peanut shells, and walnut shells. The optimal conditions for the process and the ratio of the initial components were determined. Obtained material could have promise for applications in various fields such as packaging, agriculture etc.

Key words: thermoplastic starch, biodegradable filler, sugar beet pulp, grape pomace, peanut shells, walnut shells.

POLYMERS, COMPOSITES

POSTERS

PREDICTIVE SOLVENT SCREENING FOR POLYMER ADDITIVES USING THE COSMO-SAC MODEL

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Solvent-based recycling of polymers serves as a bridge between mechanical and chemical recycling, combining the simplicity of mechanical processes with the high-quality output of chemical methods. Rather than replacing either approach, it fills the gap between them, potentially offering an effective solution for polymer purification and additive removal. The key challenge lies in selecting suitable solvents to effectively dissolve the main polymer while removing minor polymer components and additives. Additive extraction can be achieved using an anti-solvent that selectively dissolves additives while being a poor solvent for the polymer. Given the vast number of commonly used additives, experimental screening of all possible solvent candidates is impractical. Therefore, predictive thermodynamic models are essential for identifying suitable solvents. Initially, Hansen solubility parameters were used to narrow down potential candidates, but this approach was insufficient due to limited data availability and its inability to capture the chemical complexity of additives. Instead, we applied the COSMO Segment Activity Coefficient (COSMO-SAC) model, an excess Gibbs energy model that relies solely on quantum-mechanically derived σ-profiles and a few universal parameters. Solubility was assessed through (i) Solid-Liquid equilibrium calculations and (ii) ranking solvents based on activity at infinite dilution. Additionally, we addressed the challenge posed by the lack of experimental melting temperature data for complex additives (e.g., pigments) and its impact on solubility predictions. We argue that evaluating multiple descriptors offers a more comprehensive understanding of solubility rather than relying solely on the activity coefficient at infinite dilution. As one of the first studies to apply COSMO-SAC specifically to polymer additives, we demonstrate its predictive power by comparing model predictions to available experimental data from the literature.

UPCYCLING OF PLASTICS AND COMPOSITES BY THE FRACTIONATION METHOD

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This work reports on the new method of upgrading (i.e., upcycling) polymers by the fractionation method. The aim of the fractionation method is to upgrade plastics by removing degraded and short chains or by separating polymer composite materials e.g.: multilayer packaging or textiles. One enriched-valuable fraction and the second- the minor one: waste polymer material, short and broken polymer chains. The goal is to achieve the highest quality of upcycled polymers comparable with the properties of the virgin polymers. Our goal is to contribute with a feasible solution on plastic pollution problem and streamline recycling processes. The experiments were performed using our in-house-built apparatus with an automatized control. We have examined many polymer-solvent systems to enrich our data library about rheological properties and turbidity. We examined experimental measurements and systematic investigations. Measurements were taken under different conditions (temperature, pressure, solvent). As a precursor to fractionation experiments were done screening turbidimetry measurements. We observed a gel formation and changes in viscosity of polymer-solvent mixtures. Our outcome was evaluation system turbidity. These experiments were a key point used in fractionation. We performed fractionation experiments with pure polymer to upgrade polyolefin sample. The upgraded polymer chain length distributions were investigated with gel permeation chromatography (GPC), differential scanning calorimetry (DSC). The DSC is a quick method for fast determination of resulting polymer crystallinity changes. We also employed the Raman spectroscopy technique to analyze separated polymers from multilayer packaging, where we can clearly see separated polymer fractions.

Currently, our work is based on separation multicomponent plastic packaging and textiles. Textiles are mostly fabricated from COT/PES or COT/PA fibers, where both polyesters and polyamides are hard to dissolve in environmental-friendly solvents. They constitute a significant challenge in the field of plastic recycling. Thus, we see a great potential in future fractionation process of multilayers.

TRIBOLOGICAL PROPERTIES OF MATERIALS FOR ADDITIVE TECHNOLOGIES

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In recent years, various 3D printing technologies have been developed, with two of the most common methods, SLA (stereolithography) and FDM (Fused Deposition Modelling), presenting specific challenges and opportunities in the field of tribology. SLA printing focuses on surface smoothness and high resolution, leading to reduced friction under low loads, but the limited mechanical strength of the materials can be a challenge for applications exposed to high wear. In contrast, FDM printing, based on the layering of thermoplastic materials, shows greater variability in mechanical properties depending on the materials used and the printing settings. These materials, which typically have higher strength and hardness, can exhibit varying tribological behaviour, such as higher friction and wear depending on the print geometry and layer orientation. This study examines the influence of different materials and printing technologies on tribological properties and identifies key factors that affect friction and wear.

TERMOOXIDATION OF NATURAL RUBBBER WITH IRON ADMIXTURES

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Natural rubber is a key raw material widely used in industrial applications. Over prolonged use, it undergoes degradation due to oxygen, a process further accelerated by mechanical stress, elevated temperatures, and ultraviolet radiation. This interaction with oxygen leads to the formation of free radicals from unsaturated polymer chains, resulting in the gradual breakdown of the material. The degradation process can be further intensified by the presence of specific compounds known as 'rubber poisons.' These catalytic agents include transition metals such as iron, cobalt, copper, and manganese. Iron, which is commonly found in both nature and living organisms, was analysed in this research for its interaction with the structure of natural rubber. The objective of this study was to investigate the effect of iron (II) compounds on the degradation mechanisms of natural rubber and to enhance the understanding of the factors influencing its durability and properties.

HYDROFILNÍ EPOXIDOVÁ PRYSKYŘICE A JEJÍ VLASTNOSTI

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Epoxidové pryskyřice jsou jednou z nejuniversálnějších skupin polymerů, a to díky možnosti vytvrzení širokým spektrem látek s různými vlastnostmi. Právě výběr konkrétního síťovadla má stěžejní vliv na výsledné vlastnosti pryskyřice. Tato možnost nastavení vlastností epoxidu pomocí vhodného síťovadla, případně použitím plniva umožňuje využití epoxidových pryskyřic i ve velmi specifických odvětvích, jakými jsou letecký průmysl, kosmonautika nebo medicína.

Tento příspěvek se zabývá hydrofilními epoxidovými pryskyřicemi na bázi Bisfenol A propoxylát diglicidyl ether vytvrzenými vodorozpustnými Jeffaminy ®. Sleduje vliv délky tvrdidla a vybraných plniv na průběh síťování vyhodnocený pomocí axiální DMA. Dále sleduje vliv vybraných plniv na některé materiálové vlastnosti, jakými jsou například rozsah zesítění, sobce vody nebo smáčivost.

EFFECT OF CHAIN LENGTH OF SATURATED FATTY ACIDS ON VULCANIZATION ACTIVATION

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Vulcanization is a key process in rubber technology. The reaction of a vulcanizing agent with a rubber hydrocarbon creates a spatial network in which macromolecules are connected by cross-links. The concentration of cross-links and their nature determine the properties of the rubber.

Zinc oxide is an important material in rubber industry, where it is used mainly as activator of sulphur vulcanization. Oxides as vulcanization activators require the presence of a sufficient amount of fatty acid to convert them into a soluble form. This work deals with the use of saturated fatty acids (myristic, lauric, palmitic and stearic) for activating sulfur vulcanization of natural rubber. The effect on the course and kinetics of vulcanization, network density and mechanical properties of vulcanizates was studied.

This article was created with the support of the NCK project for industrial 3D printing reg. N. TN02000033, which is co-financed with the state support of the Technology Agency of the Czech Republic as part of the program of the National Center of Competence.

CRYSTALLINITY CHANGE OF SEMI-CRYSTALLINE POLYETHYLENE DURING THE SORPTION OF PENETRANTS

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Polyethylene (PE) is one of the most important and widely produced polymer materials, with many areas of application. Its manufacturing is influenced by various factors, such as the applied catalyst and reaction conditions (slurry vs. gas phase). Sorption processes accompany the entire PE manufacturing process, from monomer diffusion onto catalyst active sites to diluent desorption from the final PE powder. While many studies have examined sorption processes in PE, most assume that PE crystallinity remains constant and unaffected by sorption. However, discrepancies between experimental sorption data and theoretical predictions lead us to revise this presumption. This study demonstrates that crystallinity changes occur during penetrant sorption, altering the semi-crystalline morphology of PE. Using time-domain nuclear magnetic resonance (TD-NMR), we quantify these crystallinity changes during the sorption of various gaseous and liquid penetrants. Experiments conducted from ambient temperature up to 55°C reveal the effect of elevated temperature on sorption behaviour. Furthermore, the dynamics of crystallinity changes observed through TD-NMR offer valuable insights into the diffusion processes

within polyethylene. The dynamics data complement diffusion measurements by other methods and open the possibility of investigating diffusion processes in liquid penetrants. These insights are crucial for understanding the polymerization reactions and degassing kinetics that occur during industrial production.

3D PRINTED GELLAN AND PULLULAN ENTERIC CAPSULES

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Introduction

The aim of this work was to prepare and analyze polysaccharide-based enteric capsules for targeted drug delivery to the colon. Innovative techniques were employed in their preparation, which may significantly contribute to the development of personalized medicine. This study expands the potential use of hot melt extrusion (HME) in combination with fused deposition modeling (FDM) 3D printing.

Methodology

Filaments containing 10% or 20% polysaccharide were prepared using the HME method from a homogenized mixture of hydroxypropylmethylcellulose (HPMC) and pullulan or gellan. The key extrusion process was carried out using a Noztek Touch extruder, with the resulting filaments serving as the input material for an FDM 3D printer (Prusa i3 MK3S+). The properties of the prepared biopolymer capsules were evaluated using a range of analytical and pharmaceutical methods. A dissolution test (apparatus Sotax AT7 Smart) was crucial for the study, involving capsules filled with a mixture containing caffeine as a model API. Testing was started in dissolution medium with pH 1.2 for 2 hours. The pH of the dissolution medium was increased to 6.8 for the next 22 hours of dissolution testing. Dissolution profiles were constructed, and t_{lag} values were determined.

Results

Weight analysis revealed low variability in the weights of individual capsule components, with a standard deviation not exceeding 2%. Dimensional analysis confirmed that all measurements remained within acceptable limits. Additionally, all tested capsule formulations met the requirement for acid resistance, withstanding the acidic dissolution medium for more than 2 hours. For all formulations the lag time was around 300 minutes.

Conclusion

Based on the results, it has been confirmed that the use of HME and FDM 3D printing in combination with biopolymer materials represents a promising approach in modern pharmaceutical technology. The prepared capsules have potential not only as drug delivery systems for controlled API release into the intestinal environment but also as an alternative method for fecal microbiota transplantation.

The authors thank for support of the Ministry of Education, Youth and Sports of the Czech Republic (project SGS 2025_ 006)

INNOVATIVE SOLVENT-BASED RECYCLING: CLOSING THE LOOP ON PLASTIC WASTE

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Plastic materials are indispensable, irreplaceable and their production is increasing. However, for most plastics and textiles we do not know an efficient way how to recycle them. Unfortunately, no method has yet been devised to solve the problem of increasing waste, as it is cheaper to produce new plastic than to recycle the used one. The main problem for polymer recycling are additives, which may contain heteroatoms such as chlorine, bromine, fluorine, sulphur and nitrogen in their molecule. These elements complicate known methods of polymer recycling (pyrolysis and mechanical recycling). We focus mainly on polyolefins and polyesters, as they are one of the most widely used plastics, whose recycling has not been developed to the same state-of-art as PET. This work demonstrates a new approach to close the plastic waste loop and illustrates our approach.

The experiments were carried out in the apparatus designed specifically for additives extraction, where systematic experiments help to understand and to optimize the recycling process. It is quite difficult to know what additives are in waste plastics, so we create our own samples with known additives to calibrate spectroscopic methods. We conducted experiments using own calibration samples, so that we can clearly evaluate the efficiency of the used (mixtures of) solvents and conditions. The additive-removal experimental results were then evaluated using Raman and IR spectroscopy and compared to our calibration standards. We were also removing additives from textiles by a different method than from polyolefins. Textiles were decoloured by extracting the pigment into the solvent, that was subsequently regenerated for reuse.

This work demonstrates a new approach to close the plastic waste loop and illustrates this approach on polyolefins and textiles. The goal is to develop a simple, inexpensive and sophisticated method for plastic recycling that will can be integrated into the chain of existing recycling technologies.

CARBON NEUTRALITY

LECTURES

CONDITIONS FOR CHEMICAL INDUSTRY CARBON NEUTRALITY 2050 – TECHNOLOGIES TO BE CONSIDERED

I. Souček

Svaz chemického průmyslu ČR
VŠCHT, Praha

Main technologies contributing EU transition to carbon neutrality are listed:

- Integration of alternative energy carriers and sources, including:
    - Direct and indirect electrification of chemical processes
    - Utilization of hydrogen as energy carrier
    - Small Modular nuclear Reactors (SMR)
- Integration of non-fossil carbon feedstock:
    - Waste
    - Captured CO_2
    - Biomass
- Production of low-carbon hydrogen for use as feedstock
- Process optimization
- Carbon capture and storage

The paper comments also one of the scenario describing conditions to achieve carbon neutrality of the Czech Chemical Industry by 2050. From the analyses carried out, the following main quantified outputs for the defined part of the sector for the overall period 2019 - 2050 (i.e. about 30 years) emerge:

1. **For the deployment of abatement solutions, achievement of carbon neutrality requires investments between EUR 17.2 – 28,8 billion in the period mentioned above. The analysed options differ from each other by different phasing and type of technology investment required to achieve carbon neutrality.**
2. **The industry will consume between 80 and 110 TWh of electricity. Electricity consumption for the defined part of the sector will gradually increase from 1.5 TWh to 5 - 12 TWh (depending on the selected sub-scenario).**
3. **The total biomass demand over the period is 17-21 million t, which is about 1 million t/year in the last decade of the period under review.**
4. **Over this period, 100-130 million tonnes of CO_2 will be emitted, 3.3-8.7 million tonnes of CO_2 will be captured (of which 2.6-8.5 million tonnes of CO_2 will be stored (CCS) and 0.2-0.7 million tonnes of CO_2 will be used (CCU))**

The paper contains also main legislative challenges connected with introduction of CCU technologies and RFNBO, highlighting necessity to ensure the following principles: **Circular economy, Predictability and long-term validity of the rational regulatory framework, Digitalisation and building knowledge/capabilities, Ensuring the production of safe and sustainable chemicals and … towards Climate neutrality.**

SUSTAINABLE CHEMISTRY AND THE GREEN DEAL

T. Weidlich

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Chemical technologies based on alternative and/or renewable sources will be mentioned:

- Utilization of renewable energy sources, including:
    - Biomass instead of fossil fuels in cogeneration plants for chemical industry
    - Electrification of chemical processes exploiting electricity from renewable sources
    - Utilization of high electricity demand during negative market electricity prices
- Exploitation of non-fossil feedstocks:
    - Separation and depolymerization of biopolymers from biomass-based waste (textile waste, lignin liquors, etc.)
    - Separation and conversion of biopolymers from energy crops
    - Separation and conversion of biopolymers from agriculture wastes and forestry trash
- Production of low-carbon hydrogen as reducing agent
- Process optimization
- Waste CO_2 utilization

The presentation comments availability of waste biomass, energy crops for local cogeneration plants.

The possible role of utilization of negative electricity prices on batch chemical processes will be discussed.

Advantages of combined treatment of biomass based on preliminary separation and utilization of selected biopolymers and subsequent utilization of residual biomass for energy harvesting will be compared.

The treatment of alternative feedstocks based on produced waste (plastic waste, spent tyres) will be mentioned.

The role of selected methods for wastewater treatment enabling production of utilizable sludge (adsorption using waste biomass-based sorbents, precipitation techniques, etc.) instead of degradation techniques will be argued.

Production of biobased oxiranes and exploitation of biobased phenolic compounds for CO_2 utilization producing products profitable for agronomy will be introduced.

EVALUATING THE ROLE OF HYDROGEN AS AN ENERGY CARRIER: PERSPECTIVES ON LOW-EMISSION APPLICATIONS

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The application of hydrogen in the decarbonization process remains highly relevant topic, particularly in the context of low-emission hydrogen production methods. However, it is essential to consider also other critical steps in the hydrogen supply chain, including storage, transportation and application. The integration of these steps is crucial for the effective deployment of hydrogen technologies. This study examines hydrogen applications beyond the industrial sector, with a specific focus on its role as an energy carrier. The evaluation aims to identify the most competitive technologies for near-term implementation. A comprehensive assessment is conducted based on three key aspects. Economic feasibility analyses capital and operational expenditures associated with different hydrogen production pathways. Environmental impact assesses greenhouse gas emissions related to hydrogen production, including the potential emission reductions when replacing conventional energy sources. The third aspect is technological readiness that evaluates preparedness of hydrogen alternatives for large-scale application. A concurrent assessment of these three criteria enables a data-driven and objective comparison of available hydrogen solutions. Additionally, the study examines the projected variations in key variables, such as energy prices, carbon footprints, etc., and their impact on the final evaluation. Based on the analysed data, the study provides insights into the viable prospects of hydrogen applications in the energy sector. Furthermore, the competitiveness of low-emission hydrogen is assessed in both the energy sector and industrial applications.

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DEKARBONIZÁCIA CHEMICKÉHO PRIEMYSLU ELEKTRIFIKÁCIOU PYROLÝZNYCH PECÍ

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KĽUČOVÉ SLOVÁ: dekarbonizácia, elektrifikácia, Joulov ohrev, intenzifikácia procesov, pyrolýzne pece, parné reformovanie zemného plynu, rozkladné reakcie, zhodnocovanie CO_2 .

Čistú tepelnú energiu v elektrickej forme, aktuálne potrebnú v chemickej technológii, hľadáme nielen v bežne dostupných, ale predovšetkým v obnoviteľných zdrojoch a ako nadbytočnú v jadrových elektrárňach. V prednáške prezentujem aktuálne riešenia zamerané na dekarbonizáciu chemických procesov elektrifikáciou pyrolýznych pecí. K tejto obrovskej výzve prístupujem zohľadenim najnovších alternatívnych stratégií. Ide mi predovšetkým o to, ako náhradiť teplo v súčasnosti pochádzajúceho z konvenčného spaľovania fosilnych paliv. Je potešujúce, že vďaka celosvetovému ekologickému tlaku nastal posun smerom k plynným palivám. Od uhlia, cez ropu k zemnému plynu až k vodíku. Úplná alebo čiastočná náhrana spaľovania zemného plynu vodíkom je alternativou k elektrifikácií pyrolýznych pecí.

Z porovnania vodíka so zemným plynom sú zrejmé mnohé odlišnosti. Zatiaľ čo výhrevnosť vodíka vzhľadom na objem je len tretinová. Jeho použitie v energetických systémoch, však ďaleko presahuje toto jednoduché porovnanie. Na rozdiel od zemného plynu slúži vodík predovšetkým ako čistý nosič energie, Toto dominantné postavenie ho robí nenahraditeľným z hľadiska uskladnenia a dopravy obnoviteľnej energie. Posledná charakteristika je kľúčová pre riadenie výkyvov v nepravidelných dodávkach energie z obnoviteľných zdrojov, akými sú veterná a solárna energia.

Napriek týmto výhodám a jeho jedinečným vlastnostiam, čelí širšie využitie vodíka technickým a bezpečnostným obmedzeniam. Je bezfarebný, bez zápachu a vysoko horľavý. Vodík má širší rozsah horľavosti v porovnaní so zemným plynom. Tieto vlastnosti nutne vyžadujú špecifické zaobchádzanie a najbezpečnostnejšie technológie spaľovania.

Tým, že vodík sa ukazuje ako významný energonosič s prísľubom do budúcnosti, našiel už nadštandardné postavenie i v spektre dostupných alternatívnych energií. V porovnaní so slnečnou a veternou energiou sa javí vodík oveľa flexibilnejší a operatívnejší nosič energie. A to napriek tomu, že sa vyžadujú väčšie počiatočné technologické náklady na jeho získavanie a skladovanie. Na rozdiel od biopalív ponúka vodík čistejší proces spaľovania. Bez tvorby vedľajších, hlavne tuhých spalín. Verím, že urobená analýza pomôže pochopiť zainteresovaným stranám, skutočné postavenie vodíka. V hraniciach jeho účinnosti, nákladov, a rozsahu. Ako aj zohľadnením vplyvu na životné prostredie, v porovnaní s inými energonosičmi pochádzajúcich z obnoviteľných zdrojov

Odhaduje sa, že ročná spotreba energie v chemickom priemysle je na úrovni okolo 50 EJ/r. V dôsledku toho sa vzniká a vypúšťa do atmosféry približne 5 Gt emisií oxidu uhličitého. Výroba priemyselného tepla potrebného v petrochemickom priemysle na priebeh chemických reakcií je zodpovedná za vznik približne 1 Gt emisií oxidu uhličitého. Medzi energeticky najnáročnejšie chemické prevádzky patrí: výroba etylénu, vodíka, metanolu a amoniaku. Uvedené procesy najviac prispievajú k celkovej produkcii emisií oxidu uhličitého.

Elektrická energia umožňuje rýchle, selektívne a rovnomerné ohrievanie. Ponúka vynikajúci potenciál na využitie nadbytočnej obnoviteľnej elektrickej energie a atómovej energie. Tým prináša významné možnosti na zníženie emisií oxidu uhličitého.

Vo svojej prednáške budem preto prezentovať najefektívnejšie konverzie elektrického prúdu na teplelnú energiu nielen v existujúcich, ale aj v moderných, zatiaľ výskumne riešenych termických a katalytických procesoch. Okrem elektrifikácie veľkokapacitných pyrolýznych etylénových pecí, stručne vysvetlím princípy a základy Joule-Lencovho ohrievania. Následne Jouleho ohrev porovnám s indukčným a mikrovlnovým ohrievaním. Pozrieme sa aj na niektoré vybrané elektricky ohrievané petrochemické katalytické procesy. Z porovnania vyplýva, že Jouleho ohrievanie môžeme v súčasnosti považovať za najprijateľnejší spôsob elektrifikácie. Tak je tomu napríklad pri jeho aplikácii v parnom reformovaní zemného plynu na vodík, vo FCC procesoch a pri konverzii oxidu uhličitého na cenné petrochemikále. Dotknem sa aj ďalších výziev nielen na vývoj elektrifikácie moderných procesov, ale aj príležitostí pre nové generácie elektrifikácie chemických technológií.

Stredneteplotná pyrolýza na nízkomelekulové alkény a aromáty zohráva ústrednú úlohu pri výrobe základných petrochemikálií. Pyrolýzne pece vyžadujú obrovské množstvo energie potrebnej na rozklad uhľovodíkov na alkény a aromaty. Pyrolýzne reakcie uhľovodíkov prebiehajú v rúrkových reaktoroch uložených v peciach pri teplotách okolo 830 až 850 °C. Doteraz sa takéto teploty dosahovali spaľovaním konvenčných fosílnych palív.

Cieľom mojej prezentácie je ukázať, že kontinuálna výroba základných petrochemikálií je možná použitím elektriny ako zdroja tepla. Využitím elektriny z obnoviteľných zdrojov má tak nová technológia potenciál znížiť emisie oxidu uhličitého. V porovnaní s dnes bežne používanými technológiami je tomu minimálne o 90 %. Pritom sa jedná o proces, ktorý je jedným z energeticky najnáročnejších výrobných procesov v chemickej technológii.

Demonštračná prevádzková jednotka firiem Linde, BASF a SABIC , ktorá vyrába alkény, akými sú etylén, propylén, prípadne aj vyššie alkény z nasýtených uhľovodíkových surovín je plne integrovaná do existujúcich etylénových jednotiek v Ludwigshafene. Obsluha má za cieľ sledovať čo najviac ukazovateľov, získať čo najviac dát, presných parametrov a hlavne skúseností z prevádzkovania elektrických pecí. Pozorne sleduje ich správanie pri odlišných nástrekoch reálnych východiskových surovín. Za komerčných prevádzkových podmienok sa do pyrolýznych pecí nástrekuje hlavne primárny benzín (naphtha). Osádka sa sústreďuje predovšetkým na kľúčové uzly, pretože ich fungovanie je rozhodujúce pre úspešný vývoj inovatívnej technológie. Je tomu tak od začiatku výskumu až po uvedenie elektrických pecí do priemyselnej realizácie.

V oboch samostatne elektricky vyhrievaných pyrolýznych peciach sa testujú dve odlišné koncepcie odporového vyhrevania. V prvej peci sa realizuje priamy ohrev vedením elektrického prúdu cez odporovú špirálu umiestnenú v šamotovom plášti obopínajúceho rúrkový reaktor z vysokolegovanej ocele. Zatiaľ čo v druhej peci s nepriamym ohrevom, sa využíva na pyrolýzu sálavé teplo odporových vykurovacích teliesok umiestnených vo vymurovke (stene) elektrickej pece. Do obidvoch elektricky vyhrievaných pecí sa nastrekuje spolu okolo 4 ton primárneho benzínu za hodinu. Spotrebuje sa pritom 6 megawattov obnoviteľnej energie.

Záverom poznamenávam, že zavedením elektrických zdrojov energie do ohrievacich reakčných systémov (pyrolýznych pecí) tak, aby chemické reakcie v reaktore prebiehali žiadaným smerom a v požadovom rozsahu, bez tvorby oxidu uhličitého, ktorý vzniká spaľovaním fosílnych palív, sa zaoberajú aj firmy, spoločnosti, ústavy a univerzity: Lummmus & Brasken, Lummus SRT-e Technology, Shell & Dow, ISPT (Institute of Substainable Process Technology), TNO, Air Products, SNOOC, Technip Energies Coolbrook a Eindhoven University of Technology.

Literatúra

Zheng, L., Ambrosetti, M., Enrico Tronconi, E., (2024), Joule-Heated Catalytic Reactors toward Decarbonization and Process Intensification: A Review, ACS Eng. Au, 4, 4-24.
Tiggeloven, J. L., Faaij, A.P.C., Kramer, G.J., Gazzani, M., (2023), Optimization of Electric Ethylene Production: Exploring the Role of Cracker Flexibility, Batteries, and Renewable Energy Integration, Ind. Eng. Chem. Res., 62, 16360−16382

Linde Engineering, Starbridge Academy, (2023), Discover the electric cracking furnace..., https://www.engineering.linde.com › ...

Griffin, A., Robertson, M., Gunter,Z., Coronado,A., Xiang,Y., Zhe Qiang, Z., (2024), Design and Application of Joule Heating Processes for Decarbonized Chemical and Advanced Material Synthesis, : Ind. Eng. Chem. Res.,63,19398−19417

Hydrocarbon processing, (2024), The role of clean combustion in achieving net zero: Emphasising hydrogen´s promise, September 2024

CARBON NEUTRALITY

POSTERS

POSSIBILITIES OF IMPLEMENTING CCS TECHNOLOGY IN SLOVAKIA

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Carbon Capture and Storage (CCS) is one of the most promising solutions for reducing CO_2 emissions in industry and energy production. This contribution focuses on the possibilities of CCS implementation in Slovakia by analyzing CO_2 emissions, identifying major producers, and evaluating the suitability of various industrial enterprises for adopting this technology. The study provides an overview of current CCS projects worldwide and in Slovakia, assessing the technological, economic, and legislative factors influencing their implementation. Various CO_2 capture methods, including post-combustion, pre-combustion, and oxyfuel combustion, are evaluated concerning their technology readiness level (TRL) and commercial viability. Additionally, transport and long-term storage options for CO_2 are analyzed, with particular emphasis on geological formations in Slovakia that could serve as potential storage sites. The practical part of this contribution focuses on the design of technological processes for post combustion technology before injection into the storage site. The objective is to remove undesirable components such as O_2, CO, HCl, NO_x, and SO_2, which could negatively affect the storage process, based on legislation standards for CO2 storage in EU. The proposed solutions include various separation and purification methods, evaluated in terms of technological feasibility, efficiency, and operational costs.

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INTEGRATION OF SEA WATER DESALINATION INTO AMMONIUM THIOSULPHATE PRODUCTION

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Ammonium thiosulphate (ATS) is an inorganic compound than among other applications is being used as a fertilizer. Its production process produces a significant amount of heat that can be used for sea water desalination, especially in countries that rely on desalination for drinking water production.

This contribution investigates how the heat produced during ATS production can be used for sea water desalination. There are two approaches to this problem: desalination by using steam from ATS production for direct evaporation and electricity generation from steam turbines to power reverse osmosis systems. The study evaluates thermal efficiency and energy consumption along with water recovery performance for each method while comparing the advantages and disadvantages of direct heat use and conversion of heat into electric energy. The evaporative desalination method uses steam to boil water in an evaporator whereas the RO system depends on steam turbines to generate electricity for operating high-pressure pumps. The goal of this study is to find the most efficient desalination method that achieves minimal energy waste. The research results deliver an assessment of how ATS production byproducts can enhance desalination efficiency and support environmental sustainability.

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SYNTHESIS AND PRODUCTION OF DRUGS

LECTURES

NOVINKY VE SKUPINĚ CÍLENÝCH KANCEROSTATIK - ADC PŘÍPRAVKY (ANTIBODY DRUG CONJUGATES)

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ADC přípravky jsou cílená a rychle se rozvíjející kancerostatika, která jsou na trhu od roku 2000. Jejich obecný formát zahrnuje monoklonální protilátku (mAb), nejčastěji typu IgG, na kterou jsou přes vhodný linker (kovalentní řetězec) konjugovány molekuly cytotoxického léčiva (1-8 molekul léčiva na jednu molekulu protilátky). Konjugovaná forma léčiva má výrazně nižší toxicitu než forma volná, kterou v terapii nelze užívat samostatně. Strukturně a funkčně důležitými parametry ADC přípravků jsou: sekvence aminokyselin v mAb, posttranslační modifikace mAb, charakter linkeru (štěpitelný nebo neštěpitelný) a průměrné zatížení mAb léčivem. Tyto parametry se určují hlavně strukturně-analytickými technikami, především MS, RTG difrakcí, kryoelektronovou mikroskopií a elektronovou difrakcí. Terapeutický účinek ADC přípravků spočívá v jejich schopnosti specificky cílit a proniknout do nádorových buněk, kde následně léčivo způsobí různými mechanismy jejich apoptózu. Zároveň je využíván i terapeutický potenciál samotných protilátek.
K datu 3/2025 je celosvětově registrováno 17 ADC přípravků, z toho 14 FDA + EMA, 2 Čína a 1 Japonsko. Naproti tomu 1 přípravek (Blenrep, registrace od 2019) ztratil svoji licenci u EMA i FDA v roce 2023 na základě aktuální klinické studie DREAMM-3. ADC přípravky pokrývají poměrně širokou škálu terapií onkologických onemocnění, poslední dobou však u nich dominuje vývoj přípravků pro léčbu karcinomu prsu a použití cytotoxického léčiva ze skupiny derivátů kamptothecinu (inhibitory topoisomerasy), viz Sacituzumab tirumotekan (Čína, 2024) a Datopotamab deruxtekan (FDA, 2024, EMA 2025), které cílí na antigen Trop-2.
Na ADC přípravcích lze inovovat monoklonální protilátku (mAb), linker, způsoby konjugace, léčivo, nalézat nové cílové antigeny nebo vytvářet nové formáty konjugátů. Důvodem pro inovace je zlepšení pacientského komfortu, dosažení vyšší specificity, vyhnutí se lékovým rezistencím a vedlejším účinkům a v neposlední řadě i dosažení nižších výrobních nákladů. Příkladem nových formátů ADC přípravků jsou např. bispecifické protilátky, které se vážou na dva rozdílné cílové antigeny. Zajímavá je i možnost využití dvou různých molekul cytotoxických léčiv (tzv. dual-drug ADC). Zkoumána jsou i tzv. proléčiva ADC (Probody Drug Conjugates, PDC), která mají maskována vazebná místa protilátky (nemohou se tedy vázat na nenádorové buňky) a k odkrytí těchto vazebných míst dochází až v nádorovém mikroprostředí. Dalšími novinkami jsou tzv. Protein Degrader-Antibody Conjugates (DACs) nebo Imunne-Stimulating Antibody Conjugates (ISACs). Všechny tyto nové formáty (konstrukty) jsou zatím ve fázi výzkumu.

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INCORPORATION OF BIOLOGICALLY ACTIVE SUBSTANCES INTO POLYSACCHARIDE-BASED FIBERS

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Introduction

The lecture deals with the issue of incorporating biologically active substances into polysaccharide-based fibers. The types of bonds and interactions between the biologically active substance and the fiber, what this means for the technology and what the result is are discussed using examples.

Methodology

Cotton fibers (BA) and sodium hyaluronan (HA) fibers were selected as carriers of biologically active substances. Using dyes that simulated the structure of biologically active substances, the fixation of the dye in the fiber by covalent and ionic bonding and hydrophobic interactions was studied. The obtained results lead to a method of incorporating biologically active substances into BA and HA fibers. The antimicrobial efficacy of the materials was tested by the diffusion agar method, which serves to qualitatively assess the antimicrobial effect of the tested material. Tested microorganisms: *E. coli, Pseudomonas aeruginosa, Enterococcus faecalis, St. aureus, Candida albicans*.
The efficacy of the materials on the viability and proliferation of tumor cells was studied on the neuroblastoma cell line UKF-NB-4 and the glioblastoma cell line U87.

Results and conclusions

In the third part of the lecture, the processes that lead to truly effective materials and the technological possibilities of their production will be evaluated. The result is, firstly, cotton textiles with antimicrobial properties for the production of, for example, protective clothing. And then an invention (patent CZ 310 334 B6, 2025), which concerns staple fibers of hyaluronic acid and its salt, possibly containing oxidized starch, cross-linked with temozolomide. These fibers are suitable for the treatment of brain tumors.

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(DIS)APPEARING POLYMORPH

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Most active pharmaceutical ingredients (APIs) exhibit polymorphism and can exist in different crystalline phases. Polymorphic forms vary in their physical properties such as melting point, solubility, stability, and morphology.

Hundreds of experiments are performed during polymorphic screening with the aim of preparing the most stable polymorphic form. A broad range of crystallization techniques and solvents are employed and all forms are studied in detail via several techniques.

Despite all of this, new crystalline forms can appear in later stages of product development, which is a nightmare for scientists. Moreover, the appearing polymorph is typically a more stable, lower-energy version.

We all expect consistent results when repeating a procedure. But what if, once, you repeat the process and the results are different? Welcome to the field of (dis)appearing polymorphs, a challenging and widespread phenomenon!

Perhaps the most notorious example of a (dis)appearing polymorph is that of ritonavir[1,2]. Another example is paroxetine hydrochloride, where the hemihydrate form suddenly appeared during scale-up at two sites in the UK[3,4]. The hemihydrate was not hygroscopic and exhibited better handling properties. Rotigotine has been known since the 1980s, but in 2008, an unknown and thermodynamically more stable form emerged[5,6]. Unpredictable behavior was observed at Novartis during the development of LAB687[7]. Several crystalline forms were obtained during screening and development, but as soon as the new form emerged, the old one disappeared.

There is little to no defense against this. The solution is either to discover new polymorphs or to develop new methods for producing the original polymorphs.

1. Bauer, J. *et al.* Ritonavir: An extraordinary example of conformational polymorphism. *Pharm. Res.* **18**, 859–866 (2001).
2. Chemburkar, S. R. *et al.* Dealing with the impact of ritonavir polymorphs on the late stages of bulk drug process development. *Org. Process Res. Dev.* **4**, 413–417 (2000).
3. Pina, M. F. *et al.* Identification and characterization of stoichiometric and nonstoichiometric hydrate forms of paroxetine HCl: Reversible changes in crystal dimensions as a function of water absorption. *Mol. Pharm.* **9**, 3515–3525 (2012).
4. Rakoczy, W. A. & Mazzochi, D. M. The case of the disappearing polymorph: ‘Inherent anticipation’ and the impact of SmithKline Beecham Corp. v Apotex Corp.

(Paxil®) on patent validity and infringement by inevitable conversion. *J. Generic Med.* **3**, 131–139 (2006).
5. Wolff, H.-M., Quere, L. & Riedner, J. EP 2215072 B1 (2008).
6. Breitenbach, A. EP 1490052 B1 (2003).
7. Prashad, M. *et al.* Process research and development of a MTP inhibitor: Another case of disappearing polymorphs upon scale-up. *Org. Process Res. Dev.* **14**, 878–882 (2010).

EFFECTIVE PLANNING AND EVALUATION OF CHEMICAL PROCESSES IN TAPI: DOE AND REACTION KINETICS.

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Introduction

DOE (Design of Experiments) is a statistical approach to optimizing and describing chemical reactions, which allows changes to be made to various factors simultaneously in order to find the optimal conditions for the reaction.

The description of the kinetics of chemical reactions explains the reaction mechanism.

We use both approaches at TAPI when screening and optimizing laboratory/production steps.

Methodology

At TAPI we use JMP software from SAS, which enables visual and interactive statistical analysis of data. We create/fit kinetic models using Dynochem from Mettler Toledo.

Results

Model examples will be presented in the lecture.

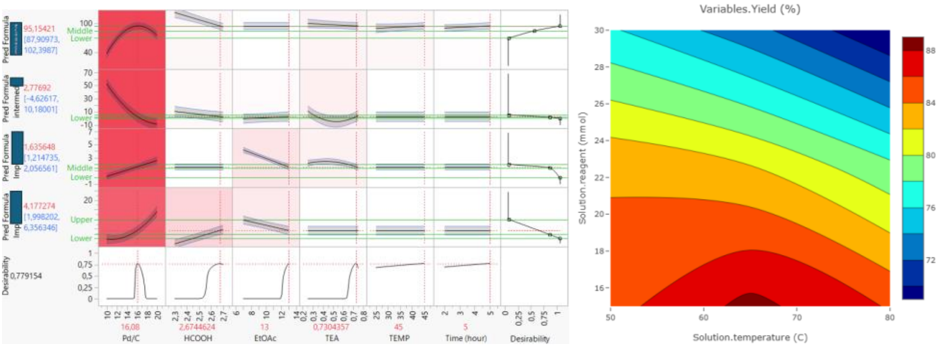

Fig.: DOE Prediction Profiler visualization; Dynochem Response Surface visualization.

Conclusions

10 years ago at Teva/TAPI DOE was a dirty word, now it is an optimization aid and an effective tool to describe reactions. Methodologies are required by FDA as part of development documents.

HOT-STAGE MICROSCOPY: EASY TOOL FOR PRELIMINARY STUDY OF API DISSOLUTION IN A FORMULATION INTENDED FOR HOT-MELT EXTRUSION

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Hot-melt extrusion is an important process for preparing solid dispersions and increasing the bioavailability of poorly soluble active substances (APIs). The resulting product is a homogeneous amorphous extrudate containing the API and a water-soluble polymer (optionally with another component). If the extrusion temperature is higher than the API's melting point, a melt of the API with the polymer will be formed; otherwise, the API must be fully dissolved in the polymer during the process. The presence of the crystalline form of the API is a problem because it can significantly affect the bioavailability of the final product. A change in the API batch having a larger particle size can, therefore, significantly affect the product quality as complete dissolution may not occur.

The behaviour of the API during melting and, thus, the dissolution of its particles, can be observed using a hot-stage microscope (HSM). This optical instrument includes a heating chamber into which a small amount of sample is placed. Typically, this device is used to observe the transitions between the solid phase and the melt (e.g., glass transition, melting point), to evaluate the particle size distribution, etc.

In this work, HSM was used to simulate the extrusion process, evaluate the equivalent particle size of API particles that were completely dissolved during the process, and determine the dissolved fraction of API. A mixture of crystalline API with particle size up to 250 µm and Kollidon® VA64 in a weight ratio of 1:4.5 was used for the experiment. The dissolution process was observed for 10 minutes at the maximum temperature at which the extrusion of this material takes place. API particle size and dissolved fraction were evaluated from two images taken at the beginning and end of the dissolution cycle.

The results showed that only particles smaller than 20 µm were fully dissolved. A linearly decreasing trend in the dependence of the dissolved fraction on particle size was observed for larger particle sizes ($d_P > 20$ µm). During the experiment, no completely dissolved particles with a size exceeding 40 µm were detected. This simple experiment confirmed why a homogeneous extrudate was not formed from this particular batch of API, as larger particles did not dissolve during the process.

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DFT-BASED VERIFICATION OF CRYSTAL STRUCTURES ACROSS THE SALT–COCRYSTAL CONTINUUM

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Pharmaceutical solid forms, such as salts and cocrystals, are essential in drug formulation. Despite differing primarily in the position of a single hydrogen atom, salts and cocrystals are subject to markedly different regulatory requirements set by the US Food and Drug Administration (FDA) [1,2]. We previously developed a computational method based on Density Functional Theory (DFT) to distinguish salts from cocrystals by optimizing artificially constructed incorrect structures [3].

In the present work, we expanded the studied dataset to 404 cocrystal models and used the rSCAN functional instead of the previously used PBE functional. The analysis confirmed that 301 of the evaluated structures were indeed cocrystals, while 87 represented salt–cocrystal continuum forms. Additionally, 16 cocrystals were classified as potential salts, in disagreement with experimental data. These problematic structures were investigated more deeply. We reproduced the crystallization process and performed data collection using single-crystal X-ray diffraction (SCXRD) for 7 of them. Complete experimental data were available for 2 problematic structures from the original authors and data re-interpretation was possible. To get the best possible hydrogen positions, we used the Hirshfeld atom refinement (HAR) method for refinement as implemented in Olex2 software and NoSpherA2.

The findings revealed that rSCAN occasionally provided unreliable results for strong hydrogen bonds; however, the discrepancies were often corrected by using better-renormalized or hybrid functionals, such as r2SCAN, PBE0, and PBE50. Among the structures exhibiting salt-like behavior, five were confirmed as salts. Our results suggest that the r2SCAN functional offers a reliable balance between accuracy and computational efficiency, particularly for O–H···N bonds longer than 2.554 Å.

1. Aitipamula, S.; Banerjee, R.; Bansal, A. K.; Biradha, K.; Cheney, M. L.; Choudhury, A. R.; Desiraju, G. R.; Dikundwar, A. G.; Dubey, R.; Duggirala, N.; Ghogale, P. P.; Ghosh, S.; Goswami, P. K.; Goud, N. R.; Jetti, R. K. R.; Karpinski, P.; Kaushik, P.; Kumar, D.; Kumar, V.; Moulton, B.; Mukherjee, A.; Mukherjee, G.; Myerson, A. S.; Puri, V.; Ramanan, A.; Rajamannar, T.; Reddy, C. M.; Rodriguez-Hornedo, N.; Rogers, R. D.; Row, T. N. G.; Sanphui, P.; Shan, N.; Shete, G.; Singh, A.; Sun, C. Q. C.; Swift, J. A.; Thaimattam, R.; Thakur, T. S.; Thaper, R. K.; Thomas, S. P.; Tothadi, S.; Vangala, V. R.; Vishweshwar, P.; Weyna, D. R.; Zaworotko, M. J., Polymorphs,

Salts and Cocrystals: What's in a Name? (vol 12, pg 2147, 2012). Cryst. Growth Des. 2012, 12 (8), 4290-4291.

2. FDA (2018) Regulatory Classification of Pharmaceutical Co-Crystals Guidance for Industry. U.S. Department of Health and Human Services Food and Drug Administration Center for Drug Evaluation and Research (CDER), February 2018 Pharmaceutical Quality/CMC Revision 1.
3. Hušák, M.; Šajbanová, S.; Klimeš, J.; Jegorov, A. (2022) Acta Crystallographica Section B. 78, 5, 781 – 788.

SYNTHESIS AND PRODUCTION OF DRUGS

POSTERS

MODULATING ANTIMICROBIAL EFFICACY THROUGH HYBRID COMPOUNDS: NOVEL LINKERS AND SCAFFOLD SWITCHING FROM ISONIAZID TO 3,5-DINITROBENZOHYDRAZIDE

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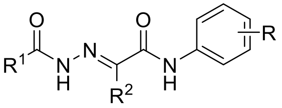
Tuberculosis and non-tuberculous mycobacterial infections present significant treatment challenges due to rising drug resistance. Building on our previous success with (*E*)-2-(2-isonicotinoylhydrazineylidene)-*N*-phenylpropanamides,[1] we expanded this chemical space by linking bioactive hydrazide pharmacophores *via* oxocarboxylic acid-based linkers (pyruvic, glyoxylic, and 4-formylbenzoic acid; Fig. 1) while incorporating various antimicrobial scaffolds[2] and additional amine derivatives. A strategic shift from the traditional isoniazid (INH) core to 3,5-dinitrobenzohydrazide, a proven building block for antimycobacterial agents, was also explored (Fig. 1) to enhance activity and circumvent common INH resistance mechanisms. The novel hydrazide-hydrazone derivatives were evaluated against a panel of mycobacteria, including drug-resistant strains, as well as against bacteria, human pathogenic fungi, for toxicity and mechanism of action. The most potent compounds exhibited MIC values as low as ≤0.25 µM against *Mycobacterium tuberculosis* and showed significant activity against *M. kansasii*. Structural modifications had a pronounced impact on antimycobacterial potency, and key structure-activity relationships (SARs) were identified, providing insights for future optimization.



R^1 = 4-pyridyl, 3,5-dinitrophenyl
R^2 = H, CH_3 or replacing 2-oxocarboxylic acid with 4-formylbenzoic acid
R = X, CF_3, alkyls, alkoxyls, arylaminosulfonyl etc.

Fig. 1. Investigated chemical space

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1. V. Pflégr, L. Horváth, J. Stolaříková, A. Pál, J. Korduláková, S. Bősze, J. Vinšová, M. Krátký; *Eur. J. Med. Chem.* 2021, 223(5), 113668.
2. V. Pflégr, K. Konečná, J. Stolaříková, J. Ősterreicher, O. Janďourek, M. Krátký; *RSC Med. Chem.* 2025,16, 767.

MODULATION OF DRUG RELEASE VIA FDM 3D-PRINTED HPMC-STARCH CAPSULES

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Introduction

Fused deposition modeling (FDM) 3D printing is a promising technique for fabricating pharmaceutical dosage forms with various drug release profiles. This study investigates hydroxypropyl methylcellulose (HPMC)-starch capsules with varying dissolution characteristics and evaluates their performance in different pH environments. By modifying formulation composition and capsule geometry, we aimed to demonstrate the potential of 3D printing for advanced drug delivery systems.

Methods

3D printing filaments were prepared using hot-melt extrusion (HME) from HPMC and starch blends in different ratios. The extruded filaments were processed into capsules using an FDM 3D printer, the Prusa i3 MK3S+. Initially, capsules of different wall thicknesses were printed from a 5% starch formulation, and based on their dissolution behavior, thick-walled capsules were subsequently printed from formulations containing 10% and 20% starch. Capsules were filled with caffeine as a model active ingredient, and dissolution testing was conducted using a Sotax AT7 Smart basket apparatus at 100 rpm in dissolution media with pH 1.2 and pH 6.8. Drug release was analyzed spectroscopically, and the obtained dissolution data were compared against each other.

Results

Thin-walled capsules were unable to reliably retain their contents for the required 2-hour period at pH 1.2, making them unsuitable for delayed-release applications. In contrast, thick-walled capsules significantly prolonged drug release, with the release time increasing as the starch content increased. At pH 6.8, dissolution was slower but followed a similar trend across all formulations.

Conclusion

The study demonstrated that 3D-printed HPMC-starch capsules enable modulation of drug release profiles through both formulation composition and capsule geometry. The observed minor pH dependency and tunable dissolution characteristics highlight the potential of FDM 3D printing for the development of personalized drug delivery systems.

Grant Support

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SOLUBILIZACE HYDROFOBNÍCH LÉČIV POMOCÍ POLYSACHARIDŮ

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Úvod

Řada potenciálních léčiv je špatně rozpustná ve vodě. Nedávno jsme vyvinuli solubilizační techniku využívající hydrofobních podstruktur biokompatibilních polysacharidů, zpřístupněných pomocí lyofilizace.[1] Nyní tak byl dříve pouze modelově popsaný proces aplikován na reálné léčivo - ciprofloxacin.

Metodika

Za účelem zpřístupnění hydrofobních domén polysacharidů byla využita metoda programově řízené lyofilizace s užitím terc-butylalkoholu coby vhodného korozpouštědla.[1] Úspěšnost přípravy systému byla potvrzena pomocí FTIR-ATR a technik fluorescenční spektrometrie.

Výsledky

Pro tuto práci byl využit hyaluronan jakožto polysacharid s předpokládanou přítomností hydrofobních domén. Jejich zpřístupnění pomocí lyofilizace bylo potvrzeno posunem absorpčního pásu v infračerveném spektru odpovídajícímu valenčním vibracím C–O vazeb ve funkčních skupinách primárních alkoholů. Změna energie této vibrace po lyfoilizaci a v přítomnosti léčiva je zapříčiněna změnou konformace sacharidu ve prospěch hydrofobního efektu v průběhu sušení. Efektivitu přípravy solubilizovatelných systému jinak špatně rozpustného ciprofloxacinu potvrdily také výsledky fluorescenční spektrometrie.

Závěr

Programově řízená lyofilizace je vhodnou metodou pro zpřístupnění hydrofobních domén polysacharidů za účelem zabezpeční rozpustnosti běžně špatně rozpustných léčiv. Výhodou této metody dále je možnost využití nativních polysacharidů bez potřeby jejich chemických modifikací.

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[1] MICHALICOVÁ, Petra, Filip MRAVEC, Miloslav PEKAŘ a Bing XU, 2017. Fluorescence study of freeze-drying as a method for support the interactions between hyaluronan and hydrophobic species. *PLOS ONE* [online]. 2017-9-8, 12(9) [cit. 2025-02-27]. ISSN 1932-6203. Dostupné z: doi:10.1371/journal.pone.0184558

Oil, gas, coal

Alternative raw materials, new technologies, biorefineries, fuels, biofuels

LECTURES

COMPATIBILITY OF CRUDE OILS AND THEIR PRODUCTS

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The compatibility of petroleum materials of different origin is a long-standing and serious problem. Because of the complexity of the colloidal system, in most cases the compatibility cannot be predicted with high reliability, particularly for materials that are subject to aging during processing, storage, or transportation to the customer. The blending of materials with different properties can also cause problems. Hence, it is not advisable to rely on only one of the standard methods when assessing compatibility. For a complete assessment, a wider portfolio of suitable analytical methods is needed. Even, some materials are so specific that an individual approach and tailor-made optimized methods need to be taken into account. This is the real reason we have dealt with this issue in great detail.

A selected series of diferent crude oils and petroleum products were subjected to mutual compatibility tests. The mixtures tested were prepared on the laboratory scale. Standard and newly developed analytical methods were used for the overall evaluation. A comprehensive approach was used to evaluate individual samples - evaluation based on the set of selected analytical indicators.

During laboratory compatibility testing, optimal blending ratios were defined for subsequent processing and final use on the industrial scale. Critical parameters were defined that could cause a problem during further processing. The incompatibility of some input materials was demonstrated, closely related to the blending ratio. In some cases, even units of mass percent played a role.

The data obtained are very important for industrial production. On their basis, it is possible to prevent various outages as clogged pumps and filters, unwanted sedimentation in storage tanks and off-spec products.

HYDROGEN PRODUCTION BY THERMO-CATALYTIC DECOMPOSITION OF SECONDARY REFINERY FEEDSTOCK

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Introduction

The increasing use of sustainable resources and the transformation of transport have an impact on energy consumption. Hydrogen is used in the energy, refining, petrochemical, food and transport industries. Hydrogen consumption reached 72 Mt in 2018 and is expected to increase exponentially with a consumption of 86 Mt in 2030 and 285 Mt in 2050. A significant change will be the replacement of traditional hydrogen sources (hydrocarbon residues, natural gas, coal) using tradition technologies as reforming (partial oxidation, steam or dry reforming) gasification and pyrolyses with "green" technologies using water electrolysis and renewable electricity. Hydrogen production by water electrolysis is energy-intensive due to the energy required to split H-O bonds (459 kJ/mol). In contrast, the energy for splitting H-S reaches 347 kJ/mol, which is 25% more energy efficient. Sulfane is produced during the sulfur removal from petroleum products by desulfurization. In refineries, it is traditionally processed into water and sulfur using the Claus process. Our project focuses on utilizing this resource for the production of valuable hydrogen while maintaining sulfur production at the ORLEN Unipetrol refinery.

Methodology

Commercial and research catalysts were characterized by selected techniques for determining the structure, composition and textural properties. The activated catalysts by sulfidation were tested in a quartz tube reactor with a fixed catalytic bed. The thermocatalytic decomposition was carried out at temperatures of 500-800 °C in a flow of 5% H_2S/N_2 and GHSV of 6 l/g/h. The catalysts activity was defined by the H_2S conversion and the H_2 amount produced. The catalysts stability was verified by the determination of metals in sulfur and also by the characterization of the spend catalyst used.

Results

A series of MoS2/Al2O3 catalyst samples prepared by different proparation methods were tested. It was found that the synthesis significantly affects the catalyst activity. It was found that the H2S conversion correlates with the increasing specific surface area of the catalyst. At 800 °C, 13% H2S conversion was achieved.

Conclusion

The catalyst positively affects the rate of the chemical reaction. At 800 °C, 4 % H_2S conversion was achieved compared to thermocatalytic decomposition, where 13 % H_2S conversion was achieved.

Acknowledgement

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CO-PROCESSING CNSL NA PREVÁDZKE HRP7 V RAFINÉRII SLOVNAFT

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Úvod

V septembri 2024 bol na prevádzke Hydrogenačnej rafinácie palív 7 (HRP7) realizovaný prevádzkový pokus na co-processing biozložky CNSL spolu so štandardnou fosílnou surovinou Pokus prebiehal pri 80 až 98 % dizajnovom výkone, pričom prístrek biozložky predstavoval v priemere 2.2 % z celkového spracovania.

Metodika

Počas trvania pokusu boli priebežne odoberané vzorky fosílnej suroviny, jednotlivých produktov a cirkulačného plynu. Taktiež bola sledovaná výťažková štruktúra produktov a kvalita cirkulačného plynu a reakčná exoterma. Vo vyrobenej nafte sa odsledovali nízkoteplotné vlastnosti. Metódou plynovej chromatografie s hmotnostným spektrometrom (GC-MS) sa stanovili produkty hydrogenácie CNSL a analýzou izotopu uhlíka 14C bol stanovený celkový obsah biozložky vo vyrobenej nafte.

Výsledky

Spracovanie CNSL malo minimálny vplyv na výťažnosť hydrogenovaného plynového oleja, ktorá klesla z 92 % na 91 % m/m. Z ostatných produktov došlo iba k miernemu zvýšeniu výťažku ľahkého benzínu a nízkotlakových plynov. Prístrek biozložky sa prejavil iba na prvom hydrogenačnom reaktore exotermickým zvýšením teploty o približne 10 °C.

V cirkulačnom plyne bolo pozorované zvýšenie obsahu metánu z 8.5 na 9.8 V/V %, sprevádzané poklesom čistoty vodíka z 85.0 až na 82.4 V/V %. Počas spracovanie CNSL nedošlo ani k zásadnej zmene nízkoteplotných vlastností vyrobeného dieslu, bod zákalu sa pohyboval v rozmedzí -1 až -2 °C a biozložka nespôsobila jeho nárast.

Pomocou GC MS boli potvrdené produkty hydrogenácie CNSL, z ktorých najväčšiu časť 1.2 m/m % tvoril n-pentadecyl cyklohexán. Analýza izotopu 14C potvrdila obsah 2.1 m/m % biozložky vo vyrobenom diesli.

Záver

Surovina CNSL sa ukázala byť ako vhodná na spracovávanie formou co-processingu na prevádzke HRP7. Prístrek CNSL výrazne nezmenil výťažkovú štruktúru a nemal negatívny vplyv na nízkoteplotné vlastnosti, zásadnejší vplyv bol pozorovaný len na čistote cirkulačného plynu. Požadované množstvo biozložky vo vyrobenom diesli bolo potvrdené analýzou izotopu 14C.

SUSTAINABLE PRODUCTION OF ADVANCED BIOFUELS VIA CO-PROCESSING OF POST-FERMENTATION CORN OIL AND STRAIGHT GAS OIL

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Abstract

Post-fermentation corn oil (PFCO), a by-product of bioethanol production from corn, contains more free fatty acids than commercial corn germ oil. This corresponds to the high acid number. PFCO contains the highest proportion of linoleic, oleic and palmitic acid. The ratio of oleic

acid/linoleic acid is in a narrow range of values from 0.49 to 0.52. The catalytic transformation of triacylglycerides on a hydrotreating catalyst and in a hydrogen atmosphere is one of the possible sources of renewable middle distillates.

Before the hydrogenation process, PFCO refining was done to remove unwanted phospholipids and reduce the metal cations in the oil. Hydrotreating of PFCO was carried out in a continuous flow tubular reactor, with a temperature range of 340-360 °C, pressure 4-5 MPa, LHSV 1 h^{-1} and ratio H_2/feedstock 450 NL/L. h in a co-processing regime with straight-run gas oil (SRGO). The catalysts used in the present study were catalysts NiMoP/Al_2O_3 and NiMoP/Al_2O_3-zeolite (sulfidic form). The decarboxylation reactions were predominant over hydrodecarboxylation. The yield of the C_{5+} fraction was 96.0 wt. %, and the n-alkane content was 83,6 wt. % due to the high free fatty acid content of 16,4 wt. %. The reaction pathway involves hydrogenation of the C=C bonds of the PFCO followed by alkane production by three different pathways: mainly decarboxylation, hydrodeoxygenation, and decarbonylation. The cracking rate was minimal in all performed experiments. The low-temperature properties of liquid products co-processing SRGO and PFCO met the normalised values for the summer period. Results show that co-processing of PFCO with kerosene and/or SRGO and hydroisomerisation can be realised on stacked-bed catalysts in one reactor. The use of corn oil from ethanol production as a bio-component in current alternative fuels has excellent potential.

Keywords
post-fermentation corn oil; advanced biofuels; hydrodeoxygenation; catalyst; co-processing

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CIRCULAR FUELS - PRODUCING EUROPE'S SUSTAINABLE AVIATION FUELS TECHNICAL ASPECTS OF THE PROJECT

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Ongoing climate change is having a negative impact on both the global economy and the lives of average citizens. The consumption of fossil raw materials, resulting in significant greenhouse gas emissions, is only accelerating these adverse changes. One way to reduce emissions of environmentally harmful gases is to use fuels produced from renewable raw materials. To intensify the development of new sustainable fuel technologies, the European Union has introduced a number of regulations, including the RED (Renewable Energy Directive) 2018/2001 of 11 December 2018. (as amended), indicating expected developments.

One of the important areas of action identified in Regulation 2023/2405 of 18 October 2023 (ReFuelEU Aviation) is the acquisition and introduction of sustainable aviation fuels (SAF) into widespread use as the most effective tool for reducing CO2 emissions in aviation (air transport in the EU is responsible for the highest CO2 emissions among transport modes, amounting to as much as 14.4% of total transport emissions).

A project exploring a novel approach to the production of SAF from waste biomass is ‘Production of sustainable aviation fuels from waste biomass by coupling of fast pyrolysis with solar energy’, abbreviated as ‘Circular Fuels’. The project is entirely EU-funded and was initiated by an international consortium of research centres and industry representatives.

The aim of the project is to produce full-value jet fuel by pyrolysis of forest and agricultural waste. Pyrolysis will take place in a reactor heated by concentrated solar energy, and the resulting bio-pyrolysis oil, after appropriate hydrogen treatment on catalysts developed for the project, will be the source of hydrocarbons for the production of finished jet fuel.

This paper will present the technical aspects of the project, indicating the tasks carried out by the consortium members.

ETG GASOLINE AND POSSIBLE WAYS OF DETERMINATION IN MIXTURE WITH FOSSIL GASOLINE

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The fuel industry is significantly influenced by the need for decarbonization. In liquid fuels, bio-components have gradually been introduced to partially replace their fossil counterparts. In diesel fuel, this was initially mainly FAME (fatty acid methyl esters), while in gasoline, ethanol was used. Over time, however, there has been a shift towards the complete replacement of these fuels with their alternatives. In Europe, the number of distributors and fuel stations offering XTL fuel as a substitute for diesel is increasing. As for gasoline, no such alternative is currently available, but a product from the EtG (Ethanol to Gasoline) process could be a promising first step. This study focuses primarily on methods for detecting and quantifying EtG in mixtures with fossil gasoline.

In this study, 19 different gasoline samples (from various countries, refineries, and with different types and amounts of bio-components) and four separate batches of EtG were used. The analytical methods employed included transmission infrared spectroscopy, FT-Raman spectroscopy, and GCxGC-MS. For data analysis, PLS, PCA, and various smoothing techniques were applied. Based on this data analysis, predictive models were developed to detect the EtG content in fossil gasoline. These models were subsequently optimized and compared with one another.

EPOXIDATION OF METHYL ESTERS FROM VEGETABLE OILS CARRIED OUT BY VARIOUS WAYS

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Current issue is searching for renewable sources for production of various materials or energy, which are presently produced from crude oil. Triacylglycerides, contained in the vegetable oils, animal fats or waste frying oils, are one of the possible renewable sources and can be transformed to ester by transesterification. The other product is glycerol, which has many applications in chemistry, food and pharmaceutical industries. The esters can be transformed to epoxides, which have many applications such as (i) bio-lubricants in means of transport (additives to oils) or (ii) raw material for bio-polymers, higher alcohols, olefins, glycols, polyesters and carbonates. These chemicals are produced from crude oil.

The epoxidation of methyl esters is carried out by hydrogen peroxide (water solution) and it is catalysed by three ways: (i) homogeneous (strong acid), (ii) heterogeneous (solid materials containing tungsten or titanium) and (iii) enzymatic (various types of lipases). All three types of catalysts will be described including advantages and disadvantages. The homogeneous is the most often applied, but the catalyst is not possible to reuse and water is used for catalyst removal. Unfortunately, the unwanted hydrolysis of epoxides can process because of the water environment. The explanation of epoxidation process by the combination of statistical analysis and quantum chemistry thermodynamic calculations is described. The heterogeneous catalyst contents tungsten or titanium, but there is a problem with stability and solvent has to be added to the reaction mixture (one liquid phase is formed). All catalysts were characterized by many methods such as the determination of metals (XRF or XPS), structure (XRD), mercury-porosimetry, UV-VIS spectroscopy, etc. The relations between outcomes from characterisation and conversion/selectivity were described. For enzymatic catalyst, various lipases are used such as *Novozym 435*, *Candida rugosa*, *Mucor javanicus*. The enzymatic catalysis offers a promising alternative to chemical catalysis, but the reaction time and especially price of enzyme are much higher than for homogeneous one. The big issue is also immobilisation of enzyme on the support.

After homogeneous catalysts, the composition of epoxidation products, i.e. dependency of various types of epoxides on reaction time, was analysed in detail (by GC-MS) at various reaction conditions. The rate constants were evaluated for each step of epoxidation.

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MIXED PLASTIC WASTE CHARACTERIZATION VIA THERMOCHEMICAL PROCESSES

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The global production and consumption of plastics has increased dramatically in recent decades, leading to an exponential increase in the production and accumulation of plastic waste. This poses a serious threat to terrestrial and marine ecosystems. Conventional waste treatment methods, such as mechanical recycling, cannot keep up with the rate of waste generation, especially for complex plastic mixtures, and do not achieve the required recycling rates. Chemical recycling is an important alternative to conventional plastic waste treatment. However, plastic waste contains numerous impurities that migrate to pyrolysis oil [1].

High-quality feedstock is essential for successful pyrolysis. The objectives of this work were to analyse plastic waste from yellow bins and assess its suitability for chemical recycling. Additionally, to identify the major impurities that would need to be further removed on the sorting line that would precede the chemical recycling technology. For these purposes, thermochemical processes like simultaneous thermal analysis (TGA, DSC), calorimetry combustion in combination with ionic chromatography (IC), elemental analysis (EA), and batch pyrolysis were used.

Literature:

[1] SNOW, J., KURÁŇ, P., KAŠPÁREK, A., LEŠTINSKÝ, P. & SUCHOPA, R. 2024. Virgin polymers via pyrolysis – A review of heteroatom removal options. *Fuel Processing Technology*, 254, 108031.

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IMPACT OF QUENCH TOWER MALFUNCTION ON STEAM CRACKER YIELDS AND PERFORMANCE

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This paper deals with the analysis of the impact of primary fractionation column malfunction on the operation of steam cracker, focusing on changes in the distillation profile, yields of key products and necessary changes in operating parameters. Damage to the column internals led to a reduced ability to separate pyrolysis products. Maintaining effective fractionation in the column required increased pyrolysis gasoline recycle. This change had a major impact on the composition of medium and heavy pyrolysis condensates.

The paper further describes the effect of pyrolysis gasoline recycle on the yields of light olefins (ethylene, propylene) and the increased formation of aromatics and carbon precipitates. During pyrolysis, naphtha containing a higher proportion of unsaturated hydrocarbons (C5 and C6 olefins) is cracked by a different mechanism than regular naphtha, which reduces the conversion to light olefins and promotes a higher coking rate in pyrolysis reactor.

Other topics include changes in the temperature profile of the furnaces, reduced steam production and strategies to optimize operation under these conditions. The results of this work are relevant not only for dealing with unplanned operational malfunctions, but also for predicting the impact of processing pyrolysis oils from waste plastics in steam crackers. Pyrolysis oil from waste plastics has a similar composition to recycled pyrolysis gasoline, which provides valuable insights for future integration of this feedstock into the steam cracking process.

EVALUATION AND OPTIMIZATION OF THE WATER QUENCH COLUMN OF UNIPETROL'S STEAM CRACKER

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The water quench tower process node represents a critical part of steam cracker's technology reducing sufficiently the temperature of cracked gas at the suction of the cracked gas compressor (CGC). If the gas is not cooled properly, the heavier hydrocarbons and additional portion of steam may overload the CGC, leading to excessive HP-steam consumption of its turbine. Every additional ton of HP-steam represents significant increase of operational costs. Furthermore, the buildup of polymer deposits within the quench tower being promoted by the increased temperature and suction pressure can compromise heat exchange efficiency, increase pressure drop, and require more frequent maintenance shutdowns.

A significant challenge in the optimization of chosen process node features the lack of direct sampling points. To address this, a process model of the main process path of the hot section has been developed in Aspen HYSYS, incorporating besides the water quench tower the primary fractionator too. This logical step was necessary in order to estimate the composition of the quench column inlet stream. The chosen approach allowed the better understanding of separation performance, potential inefficiencies and process limitations. Although sampling points are currently unavailable, they will be installed during the next planned turnaround, enabling future validation of the model and further process improvements.

A study presented in a paper explores optimization strategies, including adjustments to operating conditions, alternative cooling methods and fouling prevention techniques. A process-economic evaluation will assess the feasibility and impact of these solutions in terms of energy consumption, cost-effectiveness, and process stability. The properly made optimization allows to reduction of the HP-steam consumption having the direct positive impact on the overall CO_2 emissions, contributing to a smaller carbon footprint and improved environmental performance.

Combining computer modeling with practical process engineering solution, presented study aims to improve the reliability and overall operation of the water quench tower and compression nodes, supporting more sustainable and cost-effective ethylene production.

COKE BALANCE DURING THE DECOKING OF PYROLYSIS HEATERS

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The pyrolysis section of ORLEN Unipetrol's steam cracker unit includes eleven heaters that process four different types of feedstock. The pyrolysis heaters are operated in cycles. The operating cycle terminates with the removal of the carbon deposits (coke) produced during pyrolysis. The coke produced during the pyrolysis of hydrocarbons is a significant operational problem as its accumulation inside the reactors and transfer line exchanger reduces the efficiency of heat transfer and increases the pressure losses in the reactor. Regular decoking is necessary to maintain stable operations of the unit.

The paper describes a methodology for quantification of combusted coke based on mass balance and flue gas composition analysis. The calculation model uses flue gas composition data at time intervals from experimental sampling and allows estimation of the total amount of removed coke.

STUDY IN THE INFLUENCE OF FEEDSTOCK TYPE AND PROCESS PARAMETERS OF PYROLYSIS HEATERS ON THE FORMATION OF COKE DEPOSITS

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The ORLEN Unipetrol's steam cracker has a total of eleven pyrolysis heaters fitted with three different types of pyrolysis reactors. The cracker can process five different hydrocarbon fractions (ethane, LPG, different naphtha fractions, atmospheric gas oil and hydrocracker residue). The variety of feed-stocks in combination with different design of pyrolysis heaters (configuration of reactors, arrangement of the individual tube bundles of the convection sections, TLEs) allows the deep investigation of the coke formation and deposition at different process conditions.

The paper focuses on the quantitative aspect of coke formation for each type of feedstock. The compilation of the proper mass balance of the coke deposits is an essential condition enabling the description and understanding of the process of coke formation and deposition. The properly settled mass balance is capable to precisely quantify the amount of coke produced during the pyrolysis of individual feed-stocks. Taking into account that the proper mass balance has to cover both the amount of coke deposits carried in the stream of cracked gas and deposited on the surface of reactors tubes and TLEs. While the coke carried in the stream of cracked gas can be estimated only in limited way using the CRU situated at the quench oil loop, the amount of coke deposited in reactors and TLE can be precisely determined as the sum of the coke converted to carbon dioxide during decoking, remnants of coke remaining on the walls of TLE tubes and portion of coke released during the decoking and separated in the cyclone situated downstream the joint decoking line. The achieved results are presented for four different process cases, i.e. cracking of ethane (SMK reactors), LPG (SMK reactors), naphtha (GK6 reactors) and hydrocracker residue (SRT III reactors).

The comparison of the results enables to make general conclusions applicable to the coke deposits production at whole pyrolysis section of the steam cracker. The compilation of the balances brings an important benefit for the optimization of process parameters in case of different pyrolysis heaters, especially more precise estimation of the length of the operating cycle and decoking time. The better understanding of the coking rate makes more efficient the management of pyrolysis section, i.e. the determination of the appropriate timing of coils decoking and TLE cleaning.

NI-ZEOLITE CATALYSTS FOR METHANE SYNTHESIS: IMPACT OF SYNTHESIS CONDITIONS

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The Power-to-Gas (PtG) concept for energy and carbon storage as synthetic natural gas was first proposed by Koji Hashimoto in 1994 [1] to address long-distance electricity transmission challenges in Japan. This concept involves using electrolysis powered by renewable energy and the Sabatier reaction to synthesize methane, enabling renewable electricity distribution without the need for new infrastructure. The CO_2 produced from burning CH_4 can be recycled, contributing to carbon neutrality. In 2009, M. Sterner [2] revived the PtG concept, focusing on storing surplus renewable energy.

Our study investigates the impact of synthesis conditions on the structure and catalytic activity of Ni catalysts for methane synthesis utilizing captured CO_2 and green hydrogen. Initially, we focused on analysing zeolitic supports and finding the optimal method for incorporating active Ni centres. The standard procedure involved impregnation, calcination, and reduction. We examined the influence of different Ni sources, such as $Ni(NO_3)_2$ and Ni-acetate (NiAc). Methods of the NiAc introduction, including incipient wetness impregnation (IWI) and vacuum evaporation (VE), were compared. We also studied the effect of the zeolite support's cationic form (H^+ and NH_4^+) on Ni dispersion and the reduction conditions using pure H_2 or 5% H_2 in N_2. Additionally, we evaluated the incorporation of mesoporosity into ZSM-5 zeolites and the influence of Si/Al ratio on Ni cluster distribution and size. Finally, we tested different zeolite structures (ZSM-5, *BEA, MOR, FER).

Acknowledgement

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Reference

[1] Hashimoto, K. (1994). *Materials Science and Engineering: A*, *179*, 27-30.

[2] Sterner, Michael. *Bioenergy and Renewable Power Methane in Integrated 100% Renewable Energy Systems. Limiting Global Warming by Transforming Energy Systems: Limiting Global Warming by Transforming Energy Systems*. Vol. 14. Kassel University Press GmbH, 2009.

DETERMINATION OF GASEOUS HYDROCARBONS BY RAMAN SPECTROSCOPY

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Introduction

Qualitative analysis of natural gas, biogas, and fuel gases is essential for calculating their physicochemical properties at so-called transfer stations. Currently, analytical instruments (mainly process gas chromatographs) are used for qualitative gas determination, which require high maintenance costs, frequent calibration, and are unable to provide real-time gas composition. These shortcomings could be addressed by a non-destructive analytical method, Raman spectroscopy. The principle of Raman spectroscopy is based on the inelastic scattering of monochromatic radiation on the molecules of the sample. The resulting spectrum provides information about the rotational and vibrational transitions of the individual gas components.

Methodology

Basic hydrocarbons (methane, ethane, propane, butane) were analyzed at various pressures ranging from 2 to 10 MPa using the MonoVista CRS+ Raman spectrometer. The spectrometer consisted of a 125 mW diode laser with a wavelength of 532 nm, a monochromator with three working gratings (1800, 1500, 300 grooves/mm with a range of 350 - 1100 nm), and a cooled CCD detector with a resolution of 2000 x 256 pixels. To suppress the undesired Rayleigh scattering, three filters were used: Notch, Edge, and Bragg. A high-pressure gas cell was used for the measurements.

Results

For all tested gas samples, the main vibrational bands were identified. The effect of pressure on the shift of vibrational-rotational bands of individual gas components and changes in their intensity were also examined. Additionally, the influence of the filter on the intensity and characteristics of the measured spectra was analyzed.

Conclusion

The measurements demonstrated that with increasing pressure, some vibrational bands shifted by up to 1.6 cm^{-1}. A relationship between pressure and the width of the band at half-maximum was also identified. Additionally, the effect of the filter used on the intensity of the vibrational bands was confirmed.

TERMOMETRICKÁ TITRACE

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Termometrická titrace je analytická metoda, která využívá změny teploty během chemické reakce k určení koncentrace analytu. Tato technika je zvláště užitečná pro reakce, které nejsou vhodné pro tradiční potenciometrické nebo konduktometrické titrace.

V této přednášce se zaměříme na principy termometrické titrace, její aplikace v různých průmyslových odvětvích, převážně v petrochemického průmyslu, kde se používá například pro stanovení celkového čísla kyselosti (TAN) a celkového čísla zásaditosti (TBN). Diskutovat budeme také o nejnovějších pokrocích v technologii termometrických titrátorů, které umožňují přesnější, rychlejší analýzy a jejich automatizaci.

Společnost Metrohm, jako přední výrobce analytických přístrojů, představí své inovativní řešení v oblasti termometrické titrace, včetně praktických ukázek a případových studií. Účastníci získají hlubší porozumění o této metodě a jejího potenciálu pro zlepšení a zrychlení analytických procesů.

Metodika

Termometrická titrace

Oil, gas, coal

Alternative raw materials, new technologies, biorefineries, fuels, biofuels

POSTERS

IMPACT OF AMMONIUM USE IN HYDROTALCITE SYNTHESIS ON CATALYST ACTIVITY AND STABILITY IN BIODIESEL PREPARATION FROM WASTE COOKING OIL

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The preparation of biodiesel as an alternative fuel to commonly used fuels is an established process in technology. Its production reduces dependency on fossil fuels, thereby also decreasing environmental impact. However, a disadvantage of biodiesel production remains the use of homogeneous catalysts, which are difficult to remove from the finished product, require a large amount of water to wash out, and last but not least, produce contaminated glycerol as a byproduct. The use of heterogeneous catalysts eliminates these problems. One such catalyst is mixed oxides prepared from hydrotalcites. However, a disadvantage that has emerged in recent years is their stability during the reaction, which can lead to the leaching of metals and consequently the contamination of the product, as well as the possibility of homogeneous transesterification [1]. The most commonly observed leached element is sodium, which enters the catalyst during preparation via co-precipitation using sodium hydroxide to control pH at a constant level. In this study, hydroxide was replaced with ammonia. Two hydrotalcites were prepared: a basic Mg/Al and one with added zinc, which also serves to stabilize the structure. These catalysts were subsequently used in a batch reactor during a two-step transesterification process. Waste cooking oil from various establishments was used as the feedstock for comparison purposes. The prepared samples demonstrated very good activity in the transesterification process. Additionally, metal leaching was measured after the reaction, and the stabilization effects achieved using ammonia were compared.

Acknowledgement

This work was supported by the call for young researchers of STU to start a research career (Grant 23-09I03-03-V05)

[1] Mališová M., Hájek M., Kocián D., Malina J., Peller A., Horňáček M. The influence of various anions in Mg-Al mixed oxides on presence of sodium ions in transesterification of oil, Fuel, 319, 2022, 123781

RECYCLING OF POLYPROPYLENE WASTE FROM FOOD PACKAGING

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Plastics, a very versatile material, are applied in different sectors of industry and also in households. The global demand for plastics represents about 450 million tons per year [1]. However, a negative consequence of this consumption is the generation of plastic waste, most of which ends up in landfills. The main components of plastic waste are polyethylenes (HDPE and LDPE) and polypropylene (PP). Plastic products intended for food packaging must adhere to strict criteria regarding human health. Recyclates obtained from mechanical recycling are often unsuitable for further utilization.

Feedstock recycling is an interesting approach for utilizing plastic waste. Thermal and catalytic cracking processes, are suitable methods for producing valuable chemicals (such as ethene and propene) or fuels (like gasoline or diesel fraction). The yields and composition of fractions depend on various factors, including reaction conditions, type of reactor, residence time, and the presence or absence of a catalyst.

The work is focused on the thermal and catalytic cracking of waste PP cups in a two-stage reaction system, which consists of a batch semi-flow reactor followed by a flow reactor. The experiments were conducted at two temperatures, 420°C and 450°C. The feedstock to catalyst ratio was 1:14 by weight. Thermal and catalytic cracking were performed in the presence of an inert nitrogen flow at a rate of 60 mg/min under the same reaction conditions. A thermal cracking experiment served as a baseline to compare and determine the effect of the catalyst on the composition and yields of gas and liquid fractions. For the catalytic cracking process, was used 0.1 M acid-modified natural zeolite clinoptilolite as the catalyst. The cracking activity of clinoptilolite was confirmed at both temperatures. The yield of the gas fraction was approximately 10% higher compared to the yields from thermal cracking at 450°C.

Acknowledgement

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[1] In numbers: Europe’s mounting plastic waste problem unpacked https://www.investigate-europe.eu/posts/in-numbers-europes-mounting-plastic-waste-problem-unpacked

MODELING AND FEASIBILITY OF VARIOUS ANAEROBIC DIGESTION PLANT DESIGNS

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Anaerobic digestion offers effective and green alternative to treat various types of organic waste. The process takes place in batch or continual reactors, in which organic substrates are transformed into biogas and digestate. There are two technological approaches that differs in total solids content in feedstock – wet (<15%), dry (>20%). Produced biogas is composed of ~55% methane, ~40% carbon dioxide, nitrogen, oxygen and hydrogen sulphide. Aim of this paper is to develop a model of each available technology (continual, dry batch, wet batch) as well as unit for biogas to biomethane purification and evaluate the potential of building a new plant in Slovakia. Both dynamic and steady – state behavior of the reactor is studied. Feedstock analysis, energy integration and usability evaluation of all products are also part of the paper.

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VYUŽITIE VODÍKA AKO NÍZKOEMISNÉHO PALIVA VO VYBRANÝCH APLIKÁCIÁCH PRIEMYSLU

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Z dôvodu klimatickej krízy je potrebné nahradenie fosílnych palív v rôznych odvetviach priemyslu ekologickejšími variantami, jednou z nich by v budúcnosti mohol byť práve vodík. Podľa spôsobu výroby rozdeľujeme vodík do viacerých skupín, pričom najzastúpenejšími sú sivý, modrý a zelený vodík. Z ekologického hľadiska je hlavnou výhodou zeleného vodíka oproti iným palivám eliminácia tvorby emisií CO_2. Avšak pri jeho spaľovaní dochádza k zvýšenej tvorbe NO_x (oxidov dusíka), ktorá je zapríčinená vyššou teplotou horenia v porovnaní s napríklad zemným plynom. Z uvedeného dôvodu, ako aj kvôli rozdielnym fyzikálnym a chemickým vlastnostiam vodíka oproti zemného plynu, si spaľovanie vodíka a tiež obohateného zemného plynu vyžaduje zmeny alebo výmenu jestvujúcich horákov a tiež prepočet materiálovo tepelnej charakteristiky spaľovacích zariadení s ohľadom na ich požadovaný tepelný výkon. V tomto príspevku sa zaoberáme porovnaním energetických a environmentálnych parametrov dvoch aplikácií spaľovacích

procesov v priemysle, a to pri spaľovaní zemného plynu a po zmene palivovej základne na obohatený zemný plyn, až čistý vodík.

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BLENDED COFFEE OIL AS A POTENTIAL FEEDSTOCK FOR THE BIODIESEL PREPARATION

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Renewable energy resources, such as solar energy, wind energy, hydro-energy, and biofuels (biodiesel, bioethanol, biogas, and biomass) have been considered as a potential alternative to reduce the entire dependency on the use of fossil fuels. Amongst others, biodiesel is consistently gaining attention as a viable substitute for petroleum diesel in a near future due to its remarkable characteristics. Biodiesel production is persistently winning relevance and market due to its benefits, such as biodegradability, renewability, environmentally less toxicity, high combustion efficiency, high cetane number, high flash point, lower sulphur content, better lubrication, among others. Biodiesel is currently produced industrially by homogeneous transesterification of edible oils such as rapeseed (EU) or palm (US) oil. A more environmentally friendly and economical alternative could be the use of non-food oils, such as Camelina Sativa oil (CSO) or various types of waste oils for biodiesel preparation. However, the main disadvantage of CSO is its high content of unsaturated bonds, which is reflected in its high iodine value. This high value has a significant negative effect on oxidative stability, which raises concerns about long-term storage and also negatively affects other properties of the biodiesel prepared. A possible solution to this problem may be the blending of non-food oil with high iodine value with waste oil with low iodine value.

In this work, a blend with different ratios of *Camelina Sativa* oil and coffee oil (CO) was tested as a feedstock for transesterification with methanol at the temperature of 140 °C in batch stirring reactor, using a mixed oxide containing Mg, Al, Ni and La as a heterogeneous catalyst.

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CONVERSION OF *CAMELINA SATIVA* OIL TO FUELS IN FCC-PROCESS – STUDY IN MAT

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The work deals with the research and verification of the possibility of treatment of Camelina *sativa* oil in the process of fluid catalytic cracking (FCC) into fuels, mainly gasoline and petrochemically important fractions – C_3 and C_4 olefins. *Camelina sativa* oil was obtained by pressing of seeds of the plant *Camelina sativa*. This plant is often classed as a second-generation biofuel, as it has a non-food character. For the testing, a laboratory simulation of the FCC process - the Microactivity test (MAT), according to norm ASTM D-3907-92, was used. *Camelina sativa* oil was mixed in various ratios with the basic feed for FCC technology – desulfurized hydrogenated vacuum gas oil (HVGO). The prepared mixtures were cracked using a standard equilibrium FCC catalyst based on zeolite type Y. The dependence of the total yields of individual product fractions on the concentration of the *Camelina sativa* oil in the feed was studied and focus was aimed on the yields of the gasoline fraction and light hydrocarbon C_3 and C_4 fractions. For materials with high oxygen content such as *Camelina sativa* oil, the yields of water, inorganic gases - CO and CO_2 as well as oxygenates in liquid products were equally important. To remove these oxygenates from the liquid products, an FCC catalyst based on zeolite type ZSM-5 was added to the standard FCC catalyst. The cracking products were then analyzed by GC. The content and types of oxygenates containing liquid products were verified using GC-MS analysis. The amount of formed water was also determined in the products. The work also includes distillation curves which were based the method of simulated distillation from the liquid products GC analysis. The results of experiments confirmed the possibility of treatment of *Camelina sativa* oil as an additive to the standard FCC feed - HVGO, while increasing the yield of light products, especially the olefins in the C_3 - C_4 gas fractions. The oxygen from the bio-oil was converted by cracking into water, CO, CO_2 and products containing oxygen, which were removed by the addition of a catalyst based on zeolite ZSM-5.

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A MINI-REVIEW OF AN EPOXIDATION PROCESS OF VARIOUS VEGETABLE OILS

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Methyl esters (biodiesel) from various vegetable oils can be used as a precursor for the synthesis of epoxides. Epoxides are chemical substances with an oxygen atom bonded to two adjacent carbon atoms with a variety of applications, such as (i) lubricants, (ii) personal care products, or (iii) CO_2-capture. In this mini-review, I summarize my three-year lasting research on the synthesis of epoxides. First, an optimization study was carried out. The influence of reaction conditions (such as reaction temperature, time, or molar ratios) on the properties of epoxides was studied. A mathematical model was constructed to predict the properties of epoxides and optimize the process. Then, an analytical study was carried out. Individual reaction products were determined using GC-MS. This is a breakthrough, because no chemical standards for epoxides exist and no study had been published regarding this topic. Eventually, thermodynamic calculations were carried out for the epoxidation of *Camelina sativa* (a second-generation biofuel). This novelty allows to better understand the epoxidation process. For the future research, I would like to focus on the kinetic aspect of epoxidation.

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CATALYTIC CONVERSION OF ETHANOL TO 1-BUTANOL VIA GUERBET REACTION USING COPPER/LITHIUM-ALUMINUM MIXED METAL OXIDES

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This study focuses on the catalytic conversion of ethanol into more valuable chemical compounds, particularly 1-butanol, using heterogeneous catalysts. The Guerbet reaction in combination with copper-lithium-aluminum mixed metal oxides as catalysts was investigated as a promising pathway for ethanol transformation. The catalysts were synthesized via urea precipitation, with copper introduced either during the co-precipitation step or through post-synthetic impregnation. The catalytic experiments were conducted in a gas-phase fixed-bed reactor under a range of temperatures (300–400 °C) and pressures (1.5–10 MPa).

The significant impact of this study lies in the influence of mixed metal oxide properties on ethanol conversion and selectivity towards desired products (1-butanol, butyraldehyde, hexanol, etc.). Change in acidity and basicity, along with redox properties were factors, which played a crucial role in promoting the reaction pathway towards the desired products. Compared to conventional magnesium-aluminum catalysts, the copper-lithium-aluminum oxides proved to be more efficient, achieving up to 71 % ethanol conversion and 30% 1-butanol selectivity at reaction conditions of 350 °C and 10 MPa. This efficiency was achieved with a lower copper content, making these catalysts a noteworthy alternative to magnesium-aluminum metal mixed oxides. Despite these promising results, further optimization is required, particularly improving 1-butanol selectivity is needed.

This study contributes to the ongoing efforts to create more efficient and sustainable chemical processes, by advancing the development of heterogeneous catalysts tailored specifically for the Guerbet reaction. The findings highlight the potential of lithium-aluminum based materials for ethanol transformation, promoting the way for greener and cheaper alternatives to chemical compounds made from fossil resources.

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HYDROTREATED SPENT COFFEE GROUNDS OIL AS SAF BIO-COMPONENT

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Introduction

The world's annual coffee production is around 10 million tonnes per year. An average lipid content of 15 wt% represents about 1.5 million tonnes of non-food grade spent coffee grounds oil (SCGO) per year. Therefore, the scientific literature also addresses the issue of higher and more complex use of coffee.

Methods

The SCGO extracted with hexane has a chocolate brown colour and a characteristic coffee aroma. The crude SCGO had a high acidity (9.45mgKOH/g) and must be degummed before hydrotreatment. After extraction, it contained P 24.53; Ca 5.1; Mg 7.31; Na 1.39; K 4.94; S 35.55 mg/kg. SCGO contain triacylglycerides (54.9%), a high proportion of diacylglycerides (35.21%), monoacylglycerides (0.8%), free fatty acids (7.6%), and sterols (1.5%). Degummed SCGO mainly contains cis linoleic acid (45.4% w/w), palmitic acid (33% w/w) and oleic acid (9% w/w).

Hydrotreating of PFCO was carried out in a continuous flow tubular reactor, with a temperature range of 360-380 deg. C, pressure 4-5 MPa, LHSV 1 h^{-1} and ratio hydrogen to feedstock form 450-600 NL/L. h in a co-processing regime with n-decane or kerosine solvent. The catalysts used in the present study were $NiMoP/Al_2O_3$ and NiW/Al_2O_3-zeolite (sulfidic form).

Results

The solubility of coffee oil in kerosene, ranging from 2.5-10%vol., was successfully achieved. The hydrodeoxygenation of the coffee oil moiety, including the unsaponifiable part, was effectively completed. Minimal cracking was observed, and the C5+ yield was an impressive 98.0-99.6 wt.%. The presence of CO, CO_2, water, and propane in the gaseous fraction as products of hydrodecarboxylation, hydrodecarbonylation, and hydrodeoxygenation of glycerides and unsaponifiable fraction further validates the success of the process. The decomposition and hydrogenation of the esters of kahweol and cafestol were also evidenced by the presence of ethanol in the off-gas.

Conclusions

Coffee oil extracted from spent coffee grounds is an attractive feed for co-processing with straight-run kerosene. After degumming, it meets the recommended quality parameters for impurities in co-processing. With the tested combination of three catalysts and an injection of 2.5% by volume of coffee oil in straight-run kerosene, it reached the standard parameters for Jet A1 kerosene except for the freezing point value. The catalyst's dewaxing activity needs to be adjusted.

Acknowledgement

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WASTE UPCYCLING AND ENERGY STORAGE USING THERMAL PLASMA GASIFICATION AND PYROLYSIS

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Abstract

Among various types of thermal plasma torches, the most powerful ones are the unique self-developed high-enthalpy direct-current arc H_2O-Ar thermal plasma torch (~150 kW). This torch creates an extremely reactive conditions in a reactor, enabling the conversion (by gasification or pyrolysis) of organic materials including wastes into useful secondary raw materials. Recent materials processed include refuse derived fuel (RDF) and simulated medical waste (SMW). A major output product of this process is a synthesis gas (syngas; mainly H_2 + CO) with a lower heating value (LHV) reaching up to ~20 MJ/kg (~12 MJ/Nm^3). It has a wide range of applications in chemical synthesis, fuel production or energy conversion. Sufficient amounts of specific oxidizing agents (e.g. CO_2 or H_2O) can be used to homogenize the syngas and maximize its yield. According to our experiments and observations, the use of CO_2 as an oxidizing agent resulted in higher process efficiencies and the use of H_2O resulted in lower (carbon) soot formation (as a solid byproduct). Operating conditions and balances (such as mass, elemental and energy balance) are carefully studied, both experimentally and theoretically, with the aim of minimizing losses and improving and optimizing the process. Input fuel is typically fed at around 10 kg/h, oxidizing agents around 0-200 slm (or occasionally up to 300 slm). By converting to syngas, energy value of input material can be potentially more than doubled with thermal plasma treatment. With energy conversion efficiency reaching up to ~60%, this process is

comparable to conventional water electrolysis, one of the key approaches for green hydrogen production and renewable energy storage. Moreover, for technical practice there are wide possibilities for waste heat recovery, which can further increase the process efficiency.

Acknowledgments
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VLIV PŘÍDAVKU OLEJE Z PYROLÝZY PNEUMATIK NA VÝTĚŽKOVOU STRUKTURU PRODUKTŮ PŘI FLUIDNÍM KATALYTICKÉM KRAKOVÁNÍ

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Zpracování olejů z pyrolýzy odpadních pneumatik je v současné době atraktivní, zejména z pohledu chemické recyklace, tedy použití jako vstupní suroviny do petrochemické výroby. Výhodné je zpracování jednotlivých destilačních řezů odděleně v příslušných rafinačních technologiích. Nejproblematičtější je z tohoto pohledu zpracování destilační frakce nad 360 °C. K tomuto účelu lze využít fluidního katalytického krakování (FCC) a tím tak opět připravit vhodnou surovinu pro výrobu monomerů. Problematické mohou být některé vlastnosti pyrolýzních olejů, které ovlivňují aktivitu a životnost katalytických systémů. V této práci byl zkoumán vliv 5, 10 a 20 % hmotnostního přídavku pyrolýzního oleje z pyrolýzy odpadních pneumatik do standardní suroviny pro FCC na výtěžkovou strukturu s využitím jednotky ACE™ R+ MM. Vzhledem k vysokým obsahům síry, dusíku a kovů u pyrolýzního oleje, byl rovněž zkoumán vliv přídavku hydrokrakovaného vakuového destilátu (HCVD). HCVD slouží jako zřeďovadlo těžších rop, které jsou zpracovávány na jednotkách FCC a mohl by tedy obdobných způsobem pozitivně ovlivnit vlastnosti použitého pyrolýzního oleje. Z výsledků testů lze pozorovat, že během zpracování přídavku pyrolýzního oleje z odpadních plastů došlo ke snížení celkové konverze suroviny a ke snížení výtěžků žádaných produktů. Oproti tomu surovina obsahující přídavky pyrolýzního oleje a HCVD měla v porovnání s referenční surovinou celkovou konverzi vyšší. Z hlediska snazší dostupnosti pyrolýzních olejů s horšími vlastnostmi, lze tedy jejich možnosti zpracování pozitivně ovlivnit přídavkem HCVD.

EFFECT OF CO-PROCESSING USED COOKING OIL AND CATALYTIC HYDROCRACKING FEEDSTOCK ON PRODUCT QUALITY

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Introduction

The processing of alternative materials in current refineries has been a hot topic in recent years. Especially in the context of decarbonization and tightening emission regulations. Given the total amount of alternative materials such as used cooking oil (UCO), it is not possible to completely replace the existing production of refinery streams used to produce fossil fuels. The co-processing route therefore seems to be an attractive option to use existing equipment without the need for large investments while maintaining the capacities of the processed raw materials. UCO can therefore be used, for example, during co-processing in hydrotreating technologies, which also include catalytic hydrocracking. Here, the processing of UCO could increase the production of fractions boiling up to 360 °C, especially middle distillates.

Methodology

UCO was added in additions of 3; 6 and 12.5 wt. % to the standard processed feedstock for catalytic hydrocracking in the form of vacuum distillates. These feedstocks and the products obtained from them were evaluated using standard analytical methods. A comprehensive approach was used to assess the effect of the addition of UCO on the quality of the products.

Results

The pilot scale catalytic hydrocracking simulation under standard vacuum distillate processing operating conditions was run for 873 hours. Increasing the UCO addition in the feedstock slightly increased the conversion of products boiling up to 360 °C from 71.6 to 73.3%.

Conclusion

During the pilot simulation of catalytic hydrocracking, the possibility of processing UCO under the existing operating conditions of vacuum distillate processing was confirmed. In addition, higher conversion to the desired products boiling up to 360 °C was achieved. The addition of UCO positively influenced the increase in the product of middle distillates, for which, however, deterioration of low-temperature properties was observed.

OPTIMIZING ZSM-5 ZEOLITE FOR METHANOL-TO-GASOLINE CONVERSION: ENHANCING CATALYST LIFETIME AND SELECTIVITY

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The methanol-to-gasoline (MTG) technology [1], which converts methanol to higher hydrocarbons, is a promising alternative for gasoline production. Using methanol from renewable resources can achieve carbon neutrality and reduce fossil fuel dependency. The key to MTG is a selective and stable catalyst, typically ZSM-5 zeolites [2]. ZSM-5's structure, with linked pentasil units forming 10-ring openings, ensures high shape-selectivity for gasoline-range hydrocarbons and prevents larger molecule formation. However, strong acid sites and micropore diffusion limitations lead to fast coking and deactivation [1, 3, 4]. This research aims to develop a post-synthesis modification procedure for ZSM-5 zeolite to create a hierarchical micro-mesoporous structure with an optimal Si/Al ratio, enhancing the catalyst's lifetime and selectivity. The next goal is to scale up the catalyst synthesis to pilot scale. The modification procedure includes desilication, steaming, and dealumination, optimized for temperature, time, and leaching solution concentration. The resulting micro-mesoporous structure was characterized using HR-TEM, BET and mercury porosimetry. The effect of the structure of the micro-mesoporous catalyst on the catalyst activity and durability was tested in a fix-bed continuous flow reactor at stepwise increasing temperature and constant flow of methanol. The enhancement of micro-mesoporosity was successfully achieved by optimized modification method on lab scale.

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References

[1] Kianfar, E.; Hajimirzaee, S.; Mousavian, S.; Mehr, A. S. Microchem. J. 2020, 156, 104822.
[2] Stöcker, M. Microporous Mesoporous Mater. 1999, 29, 3-48.
[3] Ni, Y.; Sun, A.; Wu, X.; Hai, G.; Hu, J.; Li, T.; Li, G. J. Nat. Gas Chem. 2011, 20, 237-242.
[4] Sazama, P.; Dedecek, J.; Wichterlova, B.; Tvaruzkova Z.; Musilova, Z.; Palumbo, L.; Sklenak, S.; Gonsiorova O. Microporous and Mesoporous Materials 143 (2011) 87-96.

ECONOMY
OF THE CHEMICAL INDUSTRY IN NEW CONDITIONS

LECTURES

CURRENT DEVELOPMENT OF EU CHEMICAL INDUSTRY

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The paper comments current development of EU chemical industry covering:

1. Energy price comparison between EU and other regions
2. Current growth of chemical sector compared to other industrial sectors in EU
3. Capacity utilisation as a key concern and global chemical production index
4. Price index for chemicals development
5. Traded volumes development with impact of Export/Import

The EU27 chemicals industry has faced two years of economic recession (2022-2023). Compared to the USA, the gas price in Europe (Dec 2024) is 3.6 times higher, leaving Europe at a competitive disadvantage. EU27 chemicals business environment continues to face a limited demand since March 2022.

EU27 chemicals capacity utilisation is a key concern. The EU27 capacity utilisation is far below the long-term average.

The weak demand and declining business confidence continue to challenge the EU27 chemical industry. Energy is still more expensive than before the crisis and not competitive on a global scale. In spite of a production increase and a significant export improvement in volume terms, the competitiveness of the sector in Europe remains well below pre-crisis levels.

The recovery is still some way off and the demand increase will be limited due to weak economic conditions in Germany and in the USA, while the situation remains unchanged in China. The business trade environment in which European chemical companies are operating is exposed to high risk coming from additional US import tariffs.

METODIKA ANALÝZY TRHU PRO ZHODNOCENÍ TRŽNÍHO POTENCIÁLU INOVACÍ V CHEMICKÉM PRŮMYSLU

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Úvod

Správné nasměrování výzkumu a vývoje, aby přesně odpovídal očekávaným potřebám a požadavkům zákazníků a respektoval se měnící podmínky na trzích, vyžaduje provádění situačních a predikčních analýz, jejichž specifikace a návaznost jednotlivých kroků není zatím v dostupné literatuře přesně popsána. Cílem našeho příspěvku je vyplnit tuto mezeru a nastínit rámcový metodický postup pro provádění analýzy trhu umožňující zhodnocení tržního potenciálu zamýšlené inovace. Naše metodika byla využita a ověřena na konkrétním příkladu inovačního záměru v chemickém průmyslu.

Metodika

Návrh metodiky analýzy trhu byl připraven na základě literární rešerše a hloubkových individuálních rozhovorů s odborníky zabývajícími se vytvářením komerčních analýz trhu a evaluací inovačních nápadů v různých průmyslových oblastech. Připravený návrh metodiky byl prakticky aplikován při hodnocení tržního uplatnění v oblasti řešení indoorových vzduchových filtrů. Navržený postup analýzy trhu byl dle získaných praktických zkušeností upraven.

Výsledky

Koncept metodiky vychází z postupu rámcové analýzy tržního prostředí doporučovaného jako základní krok při formulaci strategie podniku. Proces byl následně transformován a upraven dle konzultací s odborníky a praktických zkušeností, aby komplexně prezentoval postup analýzy tržního prostředí v dílčích krocích analýzy makroprostředí, rámcové analýzy zákazníků a konkurence. Výsledkem je sestavení SWOT analýzy a formulace doporučení umožňujících výzkumníkům zhodnotit tržní potenciál zamýšlených inovací a zvolit správný směr následných výzkumných aktivit.

Závěr

Článek prezentuje návrh metodiky dávající výzkumníkům i ekonomům návod, jak postupovat při analýze tržního prostředí s cílem objevit potenciál tržního uplatnění zamýšlených inovací. Navržená metodika je přínosem jak pro odbornou veřejnost, tak pro komerční sféru, neboť její aplikace umožňuje přijmout vhodná opatření pro směřování výzkumných aktivit, a tedy pro rozvoj podniku i správnou evaluaci výzkumných nápadů.

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PREFERRED INFORMATION AND SOURCES FOR ASSESSING THE REPUTATION OF CHEMICAL COMPANIES AS POTENTIAL EMPLOYERS

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Introduction

This paper analyzes the information needs and preferred sources of potential employees when evaluating the reputation of chemical companies. Building on previous research on the information needs of various external stakeholder groups, this study extends the analysis to include the specific needs of the public as prospective employees. In today's labor market, where attracting and retaining talented workers is crucial for companies, it is essential to understand what information and sources the public considers important when choosing an employer.

Methodology

A primary quantitative study was conducted using an online survey with 351 respondents, who assessed the importance of different aspects of chemical companies' reputations and their preferred sources of information. Respondents were selected through purposive sampling, which, after indexing, corresponded to the demographic structure of the Czech population in terms of age and gender. The data were analyzed using statistical methods in IBM SPSS Statistics 24. This study further expands previous research by identifying specific communication preferences of companies targeting potential employees.

Results

The findings indicate that the potential employees of chemical companies consider information about health risks, salary and benefits, and career development opportunities to be the most crucial. The respondents most frequently seek this information on company websites, online job portals, and through personal accounts shared by former or current employees. Statistically significant differences in preferences regarding information sources and reputation assessment factors were identified based on age, gender, education level, expertise in chemistry, and residence near chemical plants.

Conclusion

This expanded research provides the chemical companies practical recommendations for more effective communication with potential employees. Transparency regarding working conditions, clear presentation of safety standards and career growth opportunities should be prioritized. Communication strategies should be tailored to the age, gender, and educational background of the target audience to enhance employer attractiveness and facilitate the recruitment of qualified personnel.

CIRCULAR ECONOMY IN THE CHEMICAL INDUSTRY: OPPORTUNITIES AND SOLUTIONS

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The circular economy is becoming a key concept in transforming the chemical industry towards more sustainable and efficient resource utilization. This paper focuses on concrete and functional examples of circular solutions implemented in chemical enterprises, bringing both economic and environmental benefits. We will present innovative approaches to the recycling of chemical products, such as advanced chemical recycling technologies for plastics, which enable the reuse of raw materials at the monomer level. Furthermore, we will explore closed-loop material flows in chemical operations, including solvent regeneration and the reuse of by-products in other industries. Attention will also be given to the "chemicals as a service" concept, where companies offer comprehensive solutions instead of selling chemical substances, thereby minimizing waste. The paper will also showcase examples of industrial symbiosis and asset-sharing among enterprises, leading to more efficient resource utilization and a reduced environmental footprint. Additionally, regulatory and economic challenges that may impact the broader implementation of these approaches will be discussed.

EFFICIENCY OF REVERSE LOGISTICS PROCESSES IN AN INDUSTRIAL ENTERPRISE

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The article analyzes current practices in the processing of recycling and reuse of materials and identifies key areas for improvement. The aim of the article is to propose a proposal for streamlining reverse logistics processes and optimizing product flows in the context of sustainable development of an industrial enterprise. The methods used are based on identifying ways in which reverse logistics can support sustainability, increase process efficiency and contribute to the overall improvement of supply chain management in a modern industrial environment. The conclusions and recommendations that will emerge from this article will be based on real findings from the studied enterprise. The implementation of these recommendations should not only increase the efficiency of reverse logistics processes, but also support the principles of the circular economy and contribute to reducing the environmental burden.

EXPLORING SUSTAINABLE PACKAGING INNOVATIONS: ARE BUSINESSES ADDRESSING ALL KEY ASPECTS?

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Businesses are increasingly adopting sustainable innovation strategies to minimize their environmental and societal impact. While these strategies should encompass all business processes, sustainable packaging innovations often serve as the initial step in demonstrating corporate social responsibility, particularly in the fast-moving consumer goods (FMCG) sector. This trend is driven by rising consumer awareness of packaging-related issues and growing pressure from stakeholders to ensure environmentally friendly waste management.

A key question remains whether businesses consider all aspects of sustainable packaging or focus only on specific innovations due to economic or regulatory factors. Understanding corporate preferences can highlight underutilized areas of sustainable redesign that require greater support to achieve truly effective packaging solutions. This study explores the adoption of sustainable packaging innovations in the Czech FMCG market, with a particular focus on the chemical industry (household chemicals and cosmetics). A literature review identified 26 types of packaging innovations, followed by an exploratory study involving over 200 Czech FMCG manufacturers from the food and chemical industries.

The findings reveal that manufacturers primarily concentrate on improving packaging protection, enhancing handling, and reducing material usage. Conversely, innovations involving renewable packaging materials and reusable packaging options remain less widespread. A comparison of the chemical and food industries indicates only minor differences: while food manufacturers emphasize packaging improvements to extend shelf life, the chemical industry demonstrates a more varied approach to innovation, with no single dominant trend.

SOCIAL ASPECTS OF PRODUCTION FROM THE PERSPECTIVE OF CONSUMERS

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Introduction

The sustainability of a company can be built through any pillar, i.e. in the traditional concept of the environmental, social and/or economic pillar. Recently, significant attention has been paid to the social pillar, and within it to the management of the social aspects of the company and its individual processes. When managing social sustainability, it is important for managers to take into account the requirements of individual stakeholders in a given area, including the requirements of customers. The literature has so far insufficiently addressed the perception of the importance of social aspects by customers. Therefore, primary research was conducted aimed at revealing the importance of individual social aspects associated with production processes, from the perspective of buyers of consumer chemicals and food.

Methodology

To reveal the importance of social aspects from the perspective of consumers of selected products, primary quantitative research was conducted. The respondents of the research were customers purchasing food, beverages, detergents and cosmetics, over 18 years of age. 200 responses were collected through a questionnaire in the period from December 2023 to January 2024. These responses were processed using methods of exploratory and inferential statistics.

Results

The most important social aspects in production processes were found by customers to be the working conditions and working hours, fair earnings, education and training. Analysis of differences in perception according to individual groups of respondents revealed that social aspects are more important for women than for men. The perception of importance is also influenced by the type of product produced and other characteristics of the respondents (education and age).

Conclusion

The findings of the importance of selected social aspects expands theoretical knowledge in the field of sustainability management of enterprises, especially enterprises producing food products and consumer chemical products. It also has a practical benefit, namely for managers of enterprises in industrial sectors associated with this primary research. However, the investigated social aspects do not show significant specificities of the industrial sector. Therefore, the research results are also usable by managers of production processes implemented in other enterprises.

MANAGEMENT OF SELECTED SOCIAL ASPECTS IN A CHEMICAL COMPANY THROUGH COOPERATION WITH A HEALTHCARE FACILITY

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Introduction

Social aspects, which are related to the relationship between a company and its employees, customers, communities and the wider society, focus on ensuring fair and ethical conduct of the company in the areas of human rights, working conditions, impact on the local community and relations with external partners.

Within the social responsibility in relation to the employees, it is also possible to manage the aspect of workforce regeneration. In this context, cooperation with a healthcare facility can be used. Such an area is not yet covered by the scientific literature, and for this reason the article deals with it. It states what steps should be taken when establishing a healthcare facility, which should primarily collaborate on managing selected social aspects associated with workers especially, but not only in the production processes of a chemical company.

Methodology

The article is based on a review of scientific literature and also on the results of primary qualitative research. The research activity was performed through scientific books, articles and legislative documents. The primary research was carried out in an established medical institution in the field of physiotherapy. The discovered information was compared and a proposal was made for the particular steps that should be taken when establishing a healthcare facility that will cooperate with a chemical company in managing social aspects.

Results

The results put forward a procedure that takes into account the social responsibility of the company and describes the steps necessary to establish a healthcare facility that will contribute to the management of social aspects in an already operating chemical company. These steps respect the intended cooperation with the company and include particularly a strategic marketing analysis including an analysis of legislative requirements, company requirements in the area of managing social aspects, setting a vision and a business plan.

Conclusion

In conclusion, if the individual steps described above in establishing a healthcare facility are implemented, establishing and developing cooperation with enterprises can significantly improve the management of social aspects, including aspects specific to these enterprises. The article provides rules and procedures for setting up facilities that are transferable to any field of entrepreneurship and are therefore useful for managers of both chemical companies and healthcare facilities.

DEVELOPMENT OF CORPORATE INSOLVENCIES IN THE CHEMICAL INDUSTRY

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Introduction

Companies go through different phases of the business life cycle, such as seed phase, start-up, establishment, growth, maturity, and business exit. Business termination can occur at any time and can take various forms and consequences for stakeholders. Insolvency seems to be the form with the most negative attributes and impacts on different interests' groups. Therefore, the research aimed on insolvency trends is conducted. It is exclusively focused on various areas of the chemical industry.

Methodology

To detect the insolvency trends, the quantitative research has to be conducted. First, various data sources, whether governmental or non-governmental, are collected. Second, time development and structure development according to industry branches are analysed from the absolute as well as relative point of view. It should be taken into consideration that the individual industry branches differ in their size and the number of registered business entities.

Results

The time development of corporate insolvencies in the chemical industry is described. Detected differences between the individual industry branches are pointed out. Possible reasons for the observed differences are highlighted and discussed.

Conclusion

The findings show which industry branches are more vulnerable and exposed to the higher insolvency risk. This kind of conclusion has a practical benefit for different groups of stakeholders, namely for potential investors, managers, suppliers, and customers. However, the research conducted has its limitations based on data availability. Future research tasks could be connected with international comparison and detailed exploration of reasons explaining differences between the individual industry sectors.

ACCURACY OF USING INDUSTRIAL AVERAGES IN THE CHEMICAL INDUSTRY

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Introduction

Industrial averages are frequently used for an intercompany comparison or a valuation statement. The value of industry averages can have a significant impact on the value of a business appraisal. Therefore, the research aimed on comparison of industrial averages is conducted. It is exclusively focused on various areas of the chemical industry.

Methodology

To evaluate the accuracy of using industrial averages, the quantitative research has to be conducted. First, various data sources, whether governmental or non-governmental and national or international, are collected. Second, similarities and differences in the areas of basic financial performance characteristics are analysed.

Results

Detected similarities and differences of the industrial averages employed are detected. It focuses on the areas of return, leverage, efficiency, and liquidity. Deviations between individual sectors belonging to the chemical industry are highlighted.

Conclusion

The findings show if the usage of industrial averages is accurate. This kind of conclusion has a practical benefit when the intercompany comparison should be conducted or when the averages are a basis for corporate valuations. This could have an impact on decision making of potential buyers, sellers, and valuation statements provided by professional appraisers and valuators. However, the research conducted has its limitations based on data availability.

THE CURRENT STATE OF SLOVAK WINEMAKING AS A SECTOR OF TRADITIONAL BIOTECHNOLOGY

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Slovak winemaking, as a representative of the traditional sector of so-called classical biotechnology, currently faces numerous economic challenges and opportunities, having already undergone a long and demanding journey.

This publication deals with the analysis of the current situation in the Slovak winemaking as an economic sector with a significant impact on the local economy.
As part of the analysis, we will primarily compare the development of wine production in Slovakia over the past three decades, including trends in domestic consumption and consumer quality preferences, grape prices, wine production costs, and the impact of climate change on harvests, all of which influence the industry's competitiveness.

The aim of our contribution is to provide an objective perspective on the current state and economic prospects of Slovak winemaking, identify the main challenges, and propose possible measures to strengthen its competitiveness and sustainable development.

CONSUMPTION OF ENERGY DRINKS BY CZECH GENERATION Z AND Y IN THE CONTEXT OF SOCIAL RESPONSIBILITY

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Consumption of energy drinks has increased significantly in recent years, whereas the key consumer group is in particular constituted by young people. The trend towards excessive consumption of energy drinks raises concerns not only in terms of public health, but also with regard to environmental and social responsibility as a whole. Although alternatives such as organic and sugar-free options do exist, the factors influencing choice of these drinks have not as yet been sufficiently investigated. While some studies suggest that increased education and awareness regarding the issue can lead to reduced consumption of energy drinks, the reality of consumer behaviour is often different.
This study analyses the preferences and consumer behaviour of Czech Generation Z and Y in the field of energy drinks with an emphasis on demographic factors. Quantitative research was conducted via an online questionnaire survey on a sample of 1,013 respondents. Data were processed using the statistical software package IBM SPSS

Statistics and MS Excel. Statistically significant differences were tested using a Chi-Square test and a post-hoc test.

The results show that men consume energy drinks more often than women. Generation Z exhibits a higher consumption of energy drinks than Generation Y. Consumption preferences for organic and sugar-free options are relatively low, whereas more educated groups are more frequently inclined towards sugar-free alternatives. The analysis also showed that regular consumption is more common among individuals with a lower level of education and lower awareness of health risks.

The study provides valuable insights for drinks manufacturers, policy makers and health organisations which strive to ensure regulation and education in this field. The results could also contribute towards better targeting of marketing campaigns and promotion of healthier alternatives in the drinks industry. Future research should include a deeper analysis of consumer motivations and wider international comparison.

ECONOMY AND MANAGEMENTOF RAINWATER AND WASTEWATER UTILIZATION IN TOURISM: STRATEGIES, TECHNOLOGIES, AND CURRENT STATE IN SELECTED TOURIST DESTINATIONS.

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Effective water resource management is a key aspect of sustainable tourism development. This article analyzes the economic and managerial approaches to the use of rainwater and wastewater in tourist facilities, focusing on modern technologies and strategies implemented in selected tourist destinations. It compares the current state of water recycling and reuse across different regions, identifies key challenges, and evaluates the effectiveness of applied solutions from both economic and environmental perspectives. Special attention is given to the potential of rainwater utilization to reduce potable water consumption and to innovative wastewater treatment systems. The findings highlight the importance of intelligent water resource management in the context of sustainable tourism and provide recommendations for improving water management practices in tourist facilities.

FASTER, EASIER AND MORE EFFICIENT WITH METROHM SPECTROSCOPY

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Underestimating quality control (QC) processes is a major factor leading to internal and external product failures, which have been reported to cause a loss of turnover between

10–30%. As a result, many different norms are put in place to support manufacturers with their QC processes. However, the time to obtain results and the associated costs for chemicals can be quite excessive, leading companies to implement near-infrared (NIR) and/or Raman spectroscopy in their QC processes. This presentation describes the potential of NIR and Raman spectroscopy techniques and highlights cost-saving potentials of up to 90%. NIR and Raman spectroscopy, included in the Metrohm spectroscopy portfolio, are fast, simple, and very effective non-destructive analytical techniques used for the rapid determination of multiple parameters. Information about the chemical composition and/or physical properties of liquid, paste, and solid samples can be determined in laboratories as well as continuously monitored in production. The economic benefits of these techniques will be presented in applications related to the quality control of polymers, polyols, and petrochemicals. Metrohm spectroscopic analyzers offer solutions for routine analysis along the entire production chain. The application of the latest technologies and integration with modern software futures are reflected in their speed, operability, flexible utilization, and simple automation. Do not waste your time, energy, and resources anymore. Invest in your future with Metrohm spectroscopic analyzers!

ECONOMY OF THE CHEMICAL INDUSTRY IN NEW CONDITIONS

POSTER

ESG AND PROJECT FINANCING IN THE CHEMICAL INDUSTRY

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ESG (Environmental, Social, Governance) is a comprehensive approach to evaluating companies based on their environmental and social performance and how they are governed and managed. This approach is supported by international commitments such as the Paris Agreement, but also by European Union legislation, e.g. in the form of the Corporate Sustainability Reporting Directive. Financial indicators have been and are key in making decisions about the development of companies and the financing of investment projects. Nowadays, indicators related to the impact of investment activities on the environment, society and corporate governance are also increasingly being reflected, ESG is becoming another key indicator in the assessment of investments. This paper aims to map the impact of ESG on project financing from the perspective of banks and from the perspective of companies in chemical industry. Based on structured interviews, it will be assessed to what extent the ESG approach influences the evaluation of project proposals when considering financing and insurance from the perspective of banks and insurance companies, and to what extent ESG influences the evaluation of proposals from the perspective of chemical industry companies when considering financing from internal sources or the availability of financing from external sources, e.g. in the form of bank loans. The aim is to find out to what extent these companies have had to adjust their outlook and practices related to financing towards improving their approach to sustainability.

BIOTECHNOLOGY AND BIOREFINERY

LECTURES

TWO RECYCLING APPROACHES OF POLYURETHANE FOAM USING FUNGI

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Previously applied fungus *Fusarium solani* and newly isolated fungal strain both identified as primary degrader of water-blown fully aliphatic polyurethane foam were used as source of enzymes for polyurethane recycling. Two approaches, enzymatic and microbial recycling, were tested to release and potential reuse of monomers, namely diethylene glycol and succinic acid, from polyurethane foam. Protease, lipase and esterase activity were detected in fungal growth mineral medium. Microbial recycling was based on application of fungi on polyurethane foam as growth substrate. Fungal growth was accompanied by the production of extracellular enzymes accumulating in growth medium. This approach led to release both monomers, but also partial consumption of succinic acid served as carbon and energy source for fungal growth. Tests of fungal growth on diethylene glycol and succinic acid as sole carbon and energy sources approved potential of growth on succinic acid while diethylene glycol was not utilized. Application of filtered fungi growth medium with accumulated enzymes, the bio-recycling enzymatic preparate, to polyurethane foam caused gradual release of diethylene glycol and succinic acid and their accumulation in medium as well. This approach did not lead to loss of released monomers, however, gradual loss of activity of bio-recycling enzymatic preparate was observed. Both recycling approaches have their advantages and disadvantages, and initial tests confirmed the possibility of using both methods.

VALORIZATION OF AGRICULTURAL AND FOOD WASTE IN MICROBIAL BIOTECHNOLOGY

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We are facing a substrate crisis in industrial white biotechnology. Why? Because it is unethical to use agricultural crops as substrates for the production of biofuels or bioplastic precursors when there are areas of the world where there are critical food shortages. There is a way out of this crisis and that is to use the various types of waste, which are currently undervalued, as substrates for cultivating microorganisms and obtaining value-added products. However, the use of waste is associated with various types of challenges ranging from the cleavage of difficult to use polymers into fermentable monomers (lignocellulosic complex is a typical example), to minimizing the formation of inhibitory substances during waste pretreatment and the difficult separation and purification of products from complex media. However, with knowledge of the metabolic capabilities of different types of microbial producers, valorisation of specific wastes is possible. The presentation shows a general approach to solving the problem as well as examples of specific solutions. The ideal option, which will also be discussed, would be to use raw materials in a generally biorefinery-like manner. The concept of a second-generation biorefinery will also be presented.

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POLYHYDROXYALKANOATE SYTHASES: WHAT IS KNOWN AND WHAT REMAINS TO BE DISCOVERED

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PolyHydroxyAlkanoates (PHA), microbial polyesters synthesized by various prokaryotic microorganisms, offer a solution to current challenges in the circular economy. Unlike petrochemical-based synthetic polymers, PHA are suitable for biological recycling offering sustainable, selective, and environmentally friendly plastic end-of-life options. Due to the relatively low substrate specificity of PHA synthase (PhaC) – the enzyme responsible for the synthesis of PHA in microbial cells, prokaryotes can incorporate various monomers into the polymer structure. So far, almost 140 different monomer units have been identified in naturally produced PHA polymers. Therefore, PHA are a very diverse and variable family of polymers because monomer composition significantly influences the material and technological properties of the resulting polymers. So far, four different classes of *phaC* genes and encoded synthases have been defined 20 years ago. Nevertheless, this classification may not be final as the existence of hitherto undefined classes has been already discussed. Although PHA synthases are present in many prokaryotes all over the world, their correct identification is challenging as the primary structure seems to be insufficient for the automatic identification of PHA-encoding genes and their classification. However, additional techniques considering also tertiary (3D) structure have the potential to bring desirable improvement. In our recent work, we have identified numerous synthases that were unannotated in current databases. We plan to address this limitation in the following 5 years by building a novel database aimed specifically at PHA synthases, bringing their novel classification, and characterizing every class thanks to additional experiments, including exploring the physicochemical properties of produced PHA polymers.

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BIOCONCRETE PRODUCTION USING COST-EFFECTIVE MEDIA FROM FOOD INDUSTRY BY-PRODUCTS

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The construction industry is responsible for up to 10% of global emissions. It also generates significant waste from building demolitions, particularly waste concrete fines, which currently have limited reuse options. To address this issue, we propose an innovative solution: recycling waste concrete fines through microbially induced calcite precipitation (MICP) to produce strong composite materials. However, scaling up this technology requires cost reduction, as up to 60% of the total cost is attributed to the culture medium. To tackle this challenge, we explore alternative, cost-effective sources. Feathers, which contain up to 90% protein, can serve as a culture medium. Using a machine learning model, we optimized feather hydrolysis by adjusting key parameters, including hydrolysis temperature, duration, and feather or hydroxide concentration. The optimization was based on bacterial growth metrics, specifically the lag phase duration, maximum optical density and maximum growth rate of MICP-capable bacteria *Sporosarcina pasteurii* DSM 33 and *Bacillus cohnii* DSM 6307. The resulting feather hydrolysate was used for the production of bioconcrete samples, which were analysed for their mechanical and chemical properties using X-ray diffraction, energy-dispersive X-ray spectroscopy, and scanning electron microscopy. The results demonstrated that bioconcrete produced with feather hydrolysate exhibited comparable properties to those made with commercial culture media. Furthermore, we are currently investigating other food waste sources, such as brewery yeast, spent grains, and waste meat byproducts, to further enhance the sustainability and affordability of this approach.

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THE USE OF PLANT AND ANIMAL WASTES FOR THE PREPARATION OF MEDIA FOR THE ENDOPHYTIC BACTERIA CULTIVATION

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The agricultural and food industries generate large quantities of plant and animal waste among their products, which are mostly useless or even unusable for further processing. However these materials are usually full of carbon and nitrogen sources that can still be used by other organisms, such as endophytic microorganisms, bacteria and fungi, which utilise them as an essential source of energy and building blocks for their metabolic pathways. They can use them, among other things, for the production of secondary metabolites that could be used in other areas of industry for their myriad properties. The use of waste for the production of new products is also an example of circular economy, which can lead to an increase in a company's profits or at least a reduction in the cost of environmental disposal. Plant wastes such as brewer's spent grain, animal wastes such as carp residues from fish processing, leftovers from mechanically separated chicken meat, chicken feathers and spent brewer's yeast have been used to prepare media for the cultivation of endophytic bacteria, in particular *Pantoea agglomerans* DBM 3797, which have shown the potential to become a bioactive agent in the future to promote plant growth or even protect the plants from phytopathogens.

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CHALLENGING THE PHYSIOLOGICAL TRIGGERS OF METABOLIC SHIFT IN SOLVENTOGENIC CLOSTRIDIA

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Solventogenic Clostridia are anaerobic bacteria capable of producing valuable chemicals, such as butanol and acetone, from renewable resources, making them promising candidates for sustainable industrial applications. Unfortunately, introducing raw substrates into the process often leads to insufficient metabolic shift from acidogenesis to solventogenesis, thus worse production performance. In this study, we focused on the physiological features of the culture just prior to the metabolic shift in the solventogenic strain *Clostridium beijerinckii* NRRL B-598. We have analyzed both metabolite profiles and real-time pH changes, which allowed us to precisely determine the timing and threshold value of the shift. Additional parameters measured included intracellular pH, ATP levels, NAD^+/NADH and $NADP^+$/NADPH concentrations and ratios, esterase activity, and cell culture density. The experiments were conducted in media varying in nutrient composition and with lignocellulose-derived inhibitors affecting clostridial growth and metabolism. Our findings suggest that some widely accepted theories regarding the metabolic shift—specifically ATP depletion and butyric acid accumulation might be reconsidered. A deeper understanding of the mechanisms driving this metabolic transition could help optimize conditions for large-scale, cost-effective production of bio-based chemicals from renewable feedstocks.

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BIOTECHNOLOGY AND BIOREFINERY

POSTERS

EFFECT OF ENDOPHYTIC MICROORGANISMS ISOLATED FROM WHEAT SEEDS ON GERMINATION AND PLANT GROWTH

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Endophytic microorganisms are an important part of plants. They colonize plant organs, and create complex, usually mutually beneficial interactions. Plants provide endophytes with nutrients and protection, while endophytes, in turn, produce functional metabolites that positively influence plant development. Due to these properties, endophytes are considered a potential alternative to pesticides, which, despite ensuring high agricultural yields, pose risks to human health and the environment.

This research investigates endophytic microorganisms and their potential application as a biological control of agricultural production. Endophytes isolated from winter wheat (*Triticum aestivum* L.) were used to identify and characterize properties that support germination and plant growth, with the goal of selecting microorganisms that positively affect plant development.

A total of 34 morphologically distinct bacterial strains, 2 yeast strains, and 8 filamentous micromycetes were isolated from wheat seeds. Most endophytic isolates were then identified using Gram staining, light microscopy, and MALDI-TOF mass spectrometry. Characterization of plant-beneficial properties was conducted by analyzing the production of bioactive compounds and enzymes using biochemical tests in both solid and liquid media. The results demonstrated that most bacterial and yeast isolates positively modulate plant metabolic pathways. In collaboration with the Czech University of Life Sciences Prague, the beneficial effects of endophytes were confirmed by comparing the morphological and physiological parameters of plants inoculated with selected endophytic isolates. Wheat plant development was significantly improved at the $\alpha = 0.05$ level of significance for the two isolated bacterial strains, *Pseudomonas poae* and *Pseudomonas orientalis*. However, due to large standard deviations in the measured data, a clear trend in plant growth promotion for these strains could not be confirmed.

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OPTIMIZATION OF BREWERY'S SPENT GRAIN PROCESSING FOR THE CULTIVATION OF *CLOSTRIDIUM BUTYRICUM*

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The brewing and agricultural industries today generate a significant amount of waste and by-products, including brewers' spent grains (BSG). However, BSG is a raw material that can be used as a foodstuff and has great biotechnological potential. Among other things, BSG is composed of lignocellulose and proteins, and these compounds are a promising source of nutrients such as nitrogen or carbon for the cultivation of microorganisms. The structure of lignocellulose is quite compact and difficult for microorganisms to access. It is therefore necessary to disrupt its structure so that the carbohydrates present (glucose, arabinose, xylose) can be released and subsequently utilised by the microorganisms. Lignocellulose can be degraded by several methods. One of the most environmentally friendly methods for further use in the food industry is enzymatic hydrolysis, although a pre-treatment step is often carried out before the hydrolysis itself to make the carbohydrates more accessible to the enzyme. On the other hand, there is a risk that pre-treatment will produce inhibitors derived from lignocellulose, which can subsequently have a negative effect on the growth of microorganisms.

We have optimised the hydrolysis of BSG from the point of cost-effective and efficient release of monosaccharides while minimising the presence of inhibitors such as coumaric acid, ferulic acid, furfural or hydroxymethylfurfural. After enzymatic hydrolysis, the liquid phase of the hydrolysate was used to grow *Clostridium butyricum* bacteria to verify its potential as a cultivation media.

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ISOLATING BIOLOGICALLY ACTIVE Β-GLUCANS FROM THE RED YEAST *RHODOTORULA TORULOIDES*

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β-glucans are polysaccharides known for their diverse biological activities, particularly their immunostimulatory properties, making them promising candidates for various therapeutic applications. The primary focus has been on β-glucans derived from mushrooms. However, yeast could serve as a viable alternative source offering several advantages, including higher and more consistent yields and simpler extraction processes. Nevertheless, the production of yeast-derived β-glucans remains understudied. It is essential to further optimize the extraction process for ensuring the most cost-effective production.

Several isolation procedures of β-glucans from the yeast strain *Rhodotorula toruloides* were evaluated. Namely, alkali-acid extraction method with either harsher or milder conditions with or without subsequent lipid removal using organic solvents. The glucan content was determined using enzymatic kit. The bioactive triple-helical conformation of β-glucan extracts was verified using Congo red dye.

The alkali-acid extraction method with milder conditions and further removal of the lipid content, appeared to be the most suitable isolation procedure for glucans in this specific yeast strain. The polysaccharide content reached up to 64 % (w/w) of which 78 % accounted for β-glucans. The organic solvent step was able to remove 96 % (w/w) of the present lipids. Furthermore, it was proven that the final β-glucan extract maintained its native triple-helical structure.

This research contributes to a more thorough understanding of possible isolation methods of glucans in red yeast, leading to a high yield while preserving their native bioactive tertiary structure.

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DILINOLEIC SUCCINATE BASED POLYMERS – ARE THEY GOOD ENOUGH TO OVERCOME THE EFFECTS OF BACTERIAL ACTION?

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Abstract

Today's society gives great importance to recycling and using reusable or environmentally friendly materials as an alternative to conventional plastics. However, the complete elimination of plastics from everyday life represents a significant challenge. One promising approach is to incorporate more sustainable or reusable materials such as biopolymers and bio-based polymers. However, these alternatives often face obstacles, including high acquisition costs and the need to modify the properties of polymers to achieve the desired performance characteristics. As a result, these materials have received a significant amount of attention and have been the subject of many studies and projects.

This study focuses on the degradation properties of polyester polymers, specifically poly(butylene succinate) (PBS) and its copolymers with different dilinoleic succinate

contents, when exposed to bacterial environment. Investigation revealed only modest changes in the properties of these polymers. The results obtained from gel permeation chromatography (GPC) and scanning electron microscopy (SEM) showed the main changes. Some changes were also observed by thermal analyses, including differential scanning calorimetry (DSC) and dynamic mechanical thermal analysis (DMTA).
Although the dominant process observed is abiotic degradation, the bacterial environment leads to different levels of degradation, suggesting potential applications in packaging and agriculture. Moreover, the reduced sensitivity to abiotic degradation opens up new opportunities for these polymers containing dilinoleic succinate components for future research aimed at investigating the mechanisms of bacterial and enzymatic degradation, ultimately contributing to the development of environmentally sustainable alternatives in various industries.

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DECODING POLYHYDROXYALKANOATE SYNTHASE GENES: INSIGHTS FROM DATABASE SEARCHES

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Polyhydroxyalkanoates (PHAs) are biodegradable polyesters synthesized and accumulated by prokaryotic microorganisms. The ability of these organisms to produce PHAs is encoded in their genomes. The current drawback is the hidden biosynthetic potential of prokaryotes which does not lie in the unavailability of genome sequencing and assembly, but rather in the following annotation processes. A major gap is related to PHA synthases, the enzymes responsible for PHA biosynthesis. This key enzyme in the formation of PHAs in the form of intracellular granules is being usually annotated as *phaC* or *phbC* gene. However, the recent review of PHA synthases shows that many genes are annotated as hypothetical protein coding [1]. The first step to address this gap, is using the database searches for the overview of currently available PHA synthase gene sequences. We will utilize full-text searches based on gene abbreviations and enzyme identifiers. This includes searches in Kyoto Encyclopedia of Genes and Genomes (KEGG) [2]. The number of *phaC* genes in the KEGG GENES database is currently 4320 available under the EC 2.3.1.304. Another database including *phaC* genes is Clusters of Orthologous Genes (COG) [3] currently with 1299 genes under identifier COG3243. Our work attempts to give an insight into the primary structure of PHA synthases by a combination of bioinformatics approaches to identify PHA synthase coding genes across annotated prokaryotic genomes.

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[1] Zher Neoh, S.; et al., 2022. Polyhydroxyalkanoate synthase (PhaC): The key enzyme for biopolyester synthesis. *Current Research in Biotechnology*. Roč. 4, pp. 87-101. ISSN 25902628. Doi: 10.1016/j.crbiot.2022.01.002.

[2] Minoru K., et al., 2025. KEGG: biological systems database as a model of the real world, *Nucleic Acids Research*, Volume 53, Issue D1, 6 January 2025, Pages D672–D677. Doi: 10.1093/nar/gkae909.

[3] Galperin MY, et al., 2024. COG database update 2024. *Nucleic Acids Res*. 2025 Jan 6;53(D1):D356-D363. PMID: 39494517; PMCID: PMC11701660. Doi: 10.1093/nar/gkae983.

VALORISATION OF NITROGEN-RICH FOOD WASTE MATERIALS FOR BIOMASS PRODUCTION IN BASIDIOMYCETE AND ASCOMYCETE YEASTS

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Yeasts represent a diverse group of microorganisms capable of synthesizing a wide range of nutritionally and biologically valuable compounds, including β-glucans, lipids, ergosterol, ubiquinone, and, in certain species, carotenoid pigments. A key advantage of cultivating microscopic fungi lies in their ability to utilize food industry by-products as nutrient sources, particularly carbon and nitrogen, following appropriate pretreatment.

This study aims to evaluate various industrial food waste-derived nitrogen sources—flax hydrolysate, whey protein hydrolysate, spent brewer's yeast hydrolysate, and feather hydrolysate—by assessing the resulting microbial biomass enriched with valuable metabolites. Additionally, flax oil was introduced into media as carbon source and as a supplementary nutritional stress factor. The ascomycete strain *Metchnikowia pulcherrima* and the basidiomycete strain *Rhodotorula kratochvilovae* were cultivated under controlled C/N ratios to ensure comparability of the results.

The findings indicate that both yeast strains effectively utilize food waste-derived substrates for biomass production. *R. kratochvilovae* demonstrated the highest biomass yield when cultivated on medium supplemented with feather hydrolysate as the nitrogen source (10.6 ± 0.1 g/L). *M. pulcherrima* exhibited maximal biomass production on a medium containing feather hydrolysate and flax oil (10.4 ± 0.2 g/L). Future research will focus on expanding the study to additional yeast strains and scaling up the cultivation process to a laboratory-scale bioreactor to further explore the feasibility of industrial applications

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SEPARATION AND PURIFICATION OF *MONASCUS* PIGMENTS

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Monascus pigments (MPs) are natural coloring agents produced by *Monascus* spp., with a usage history of over 2,000 years. They are widely applied in the food industry now and have promising potential for use in biomedicine, textiles, dying, and cosmetics in future. Advances in molecular biology and biochemistry have provided a detailed understanding of the biosynthetic pathways of MPs, while studies on optimizing cultivation conditions—such as media composition and fermentation parameters—have aimed to improve MPs' yield for higher economic returns. Despite their vivid colors and diverse bioactivities, MPs are typically utilized as unpurified mixtures in industrial applications due to the lack of easily accessible, purified, stable individual compounds. While mixed MPs are commonly used in food products to impart red color, they actually consist of a complex mixture categorized into three groups based on color: red, orange, and yellow. There is significant market demand for natural orange and yellow colorants as well. Furthermore, for biomedical applications, individual pigment compounds must be purified to eliminate potential interactions and enhance functional specificity. This review summarizes and compares the methodologies developed over the past decades for the isolation and purification of MPs. With advancements in these purification techniques, the potential applications of single purified MPs across various industries will be significantly expanded.

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EFFECT OF ENRICHED LIGNOCELLULOSIC WASTES AS A PRIMARY NUTRITIONAL SOURCE ON THE BIOMASS QUALITY OF SELECTED YEAST STRAINS

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Yeasts are a diverse group of microorganisms capable of producing a variety of nutritionally and biologically valuable metabolites, including a wide range of antioxidants such as carotenoids, ubiquinone, ergosterol, β-glucans, microbial lipids and others. One significant benefit of cultivating these microscopic fungi is their ability to utilize various nutrient sources, such as industrial by-products, after appropriate pretreatment of this alternative source.

The aim of this work is to optimize the cultivation conditions of selected yeasts on low-cost lignocellulosic waste materials, with the addition of microbiogenic elements (iodine, iron). The goal is to determine which form of mineral is optimally utilized by microorganisms, whether it is possible to fortify the biomass with multiple elements simultaneously, and how much of each element accumulates in the biomass when combined with the selected waste material. The strain *Metchnikowia pulcherrima* and the strain *Rhodotorula toruloides* were cultivated under controlled C/N ratios to ensure comparability of the results. Metabolites contained in biomas, were analyzed by various laboratory techniques, included gas chromatography (GC) and high performance liquid chromatography (HPLC).

According to the results of the study so far, we can confirm that both strains utilize the waste nutrient sources. The highest biomass yield was recorded in the *R. toruloides* strain when hydrolyzed brewery spent grain was used in combination with sodium iodate (13.15 mg biomass/ml medium). In the *M. pulcherrima* strain, the highest biomass yield was recorded when coffee hydrolysate was used as a nutrient source and ferric chloride was added (9.5 mg biomass/ml medium).

The results of this work can provide valuable informations with application in industrial biotechnology of enriched yeasts biomass and reduce their economic demandingness and at the time provide aid with ecological disposal of selected waste materials.

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CAN HYDROGEN AND BIOPLASTICS BE COMBINED?

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With the rapid development of industry and its deepening impact on climate change, interest in the possible use of alternative energy sources has been growing in recent years. On of suitable type of renewable energy is the production of combustible gases such as methane or hydrogen. The advantage of hydrogen is that when burning it, only water vapour is produced [1].

One of the possible avenue for hydrogen production could be biotechnological production using microorganisms capable of producing it using carbohydrate-rich waste materials. Among the promising hydrogen producers are bacteria of the genus *Clostridium*. These bacteria, which are strict anaerobes, produce hydrogen acetic and butyric fermentation, using organic matter as the primary source of hydrogen and energy. These organic substrates include glucose and other hexoses, lactose, sucrose, starch, etc [2].

This work focused on the description of hydrogen production by the anaerobic bacteria *Clostrodium butyricum* and *Clostridium tyrobutyricum* with a focus on the optimal conditions for biohydrogen production such as culture time, suitable medium, etc. Furthermore, first part of this work was focused on the development of a suitable apparatus for the collection of the produced gas mixture followed by the analysis of the composition of produced gas mixture by Hiden QGA ("quantitative gas analysis"). The second part of this work was aimed at verifying the possibility of biotechnological treatment of the liquid fraction of hydrogen production. These supernatants were analyzed by ion chromatography (IC) to determine the organic acid content. Following this, the use of this material as a substrate for the production of polyhydroxyalkanoates by already known PHA producers was verified.

References

[1] D. Liu, Bio-hydrogen production by dark fermentation from organic wastes and residues. . Miljoevej, 2008, p. 60

[2] H. Argun, F. Kargi, I.K. Kapdan, Microbial culture selection for bio-hydrogen production from waste ground wheat by dark fermentation, Internation Journal of Hydrogen Energy, p. 34

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ANIMAL WASTE AS A SOURCE OF VALUABLE PRODUCTS

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Hydrolysis of various types of animal waste is a practical method for processing difficult-to-use raw materials. In addition, our system using malic or citric acid to hydrolysis initiation does not produce unwanted salts, so it is in line with environmental sustainability.

Animal hydrolysates are widely used in various areas due to their elemental composition, content of fatty acids, acylglycerides, amino acids as well peptides.

In agriculture, they can be used as fertilizers or bio-stimulants that support the growth of the root system, aerial biomass of plants, support flowering and increase seed yields. This stimulating effect was verified and confirmed in field trials with spring barley and winter wheat planting. Field trials were conducted according to the GEP (Good Experimental Practice) methodology and were sown on an area of 10 m^2 for each variant in 5 randomized replicates. Hydrolysates can also protect plants from excessive sunlight and reduce water evaporation. They are also recently tested for plant protection against ungulate bites. Moreover, the residual solid fraction can be advantageously used not only in compost, but also in vermicompost.

It has also been verified that hydrolysates stimulate the growth of beneficial bacteria in the soil by up to 3 orders of magnitude, which contributes to its quality.

Keywords: hydrolysates, animal waste, bio-stimulation.

Acknowledgement
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VÍCE NEŽ JEN P(3HB): TERMOFILNÍ BAKTERIE RODU *ANEURINIBACILLUS* JAKO ZDROJ NETRADIČNÍCH PHA KOPOLYMERŮ

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Úvod

Polyhydroxyalkanoáty (PHA) jsou mikrobiální polyestery, které kombinují vlastnosti běžných plastů s biologickou rozložitelností, biokompatibilitou a netoxicitou, což je činí atraktivními jako možnou alternativu k petrochemickým plastům. Nejčastěji produkovaným PHA polymerem je poly(3-hydroxybutyrát) (P(3HB)) – homopolymer, který je však kvůli své vysoké krystalinitě křehký a nepružný. Zlepšení jeho mechanických vlastností lze dosáhnout integrací dostatečně strukturně odlišných PHA monomerů do polymerního řetězce, čímž dochází ke snížení krystalinity a zvýšení elasticity. Tyto PHA materiály se svými vlastnostmi více přibližují syntetickým plastům a rozšiřují možnosti jejich praktického využití.

Metodika

Termofilní bakterie rodu *Aneurinibacillus* byly kultivovány v přítomnosti vybraných prekurzorů (laktony/dioly). Získaná biomasa byla analyzována plynovou chromatografií (GC-FID) k identifikaci produkovaných PHA polymerů. Následně byly polymery extrahovány a charakterizovány pomocí různých analytických metod, jako je nukleární magnetická rezonance (NMR), infračervené spektroskopie (FT-IR), diferenciální skenovací kalorimetrie (DSC), chromatografie s víceúhlovým rozptylem světla (SEC-MALS) a dalších technik s cílem určit jejich materiálové vlastnosti.

Výsledky

Bakterie *Aneurinibacillus* úspěšně syntetizovaly PHA kopolymery obsahující monomery jako 4-hydroxyvalerát (53,1 mol. %), 5-hydroxyvalerát (44,2 mol. %), 4-hydroxybutyrát

(80,2 mol. %) a 4-hydroxyhexanoát (11,5 mol. %). Začlenění těchto monomerů do struktury polymeru vedlo k výraznému snížení krystalinity, zvýšení elasticity a celkovému zlepšení fyzikálně-chemických vlastností materiálu.
Kromě toho byl úspěšně syntetizován unikátní PHA kopolymer obsahující 4-hydroxy-2-methylbutyrát (4H2MB), přičemž jeho obsah dosáhl až 11,14 mol. %. Změny v termálních vlastnostech a struktuře byly potvrzeny řadou technik, jako je DSC a FT-IR. Podle dostupné literatury se jedná o první případ produkce 4H2MB divokým kmenem.

Závěr

Termofilní bakterie rodu *Aneurinibacillus* se prokázaly jako spolehliví producenti zajímavých PHA kopolymerů. Tato schopnost je pravděpodobně výsledkem činnosti velmi nespecifických PHA syntáz, které těmto bakteriím umožňují využívat různé prekurzory a syntetizovat širokou škálu zajímavých PHA kopolymerů, které mohou lépe konkurovat tradičním plastům než klasický P(3HB).

TRANSCRIPTOMIC INSIGHTS INTO ACID CRASH AND NON-SPORULATING CULTIVATIONS OF *CLOSTRIDIUM BEIJERINCKII* NRRL B-598

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Various bacterial strains are studied for their remarkable ability to thrive in diverse conditions and produce substances with great biotechnological potential. One such strain is *Clostridium beijerinckii* NRRL B-598, known for its ability to produce hydrogen and butanol during acetone-butanol-ethanol (ABE) fermentation. To better understand the ABE fermentation pathway at the gene level, several RNA-Seq datasets have been published, accompanied by transcriptomic studies focusing on standard and butanol-shocked cultivations.
Here, we present two new RNA-Seq datasets: the first was obtained from a cultivation in which an acid crash phenomenon was observed, while the second was acquired from a non-sporulating cultivation. Both datasets consist of six time-points selected to capture key stages of ABE fermentation and enable direct comparison with data from standard cultivation. This enabled us to perform differential expression analysis and gene ontology enrichment analysis, identifying changes in expression profiles of genes related to the ABE fermentation pathway. Additionally, we uncovered significantly enriched molecular functions and biological processes associated with the acid crash event and the non-sporulating culture. Our findings provide new insights into the regulatory mechanisms of *Clostridium beijerinckii* NRRL B-598, contributing to a deeper understanding of its metabolic adaptation and biotechnological potential.

IMPACT OF GENETIC DELETIONS ON THE BIOTECHNOLOGICAL POTENTIAL AND STRESS ROBUSTNESS OF *CALDIMONAS THERMODEPOLYMERANS* IN PHA PRODUCTION

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Bacterial polyhydroxyalkanoates (PHA) represent an interesting source of natural biodegradable substances that are finding applications in an increasing number of industrial fields. They have attracted attention mainly due to their properties similar to petrochemical plastics. Promising producers are thermophilic bacteria, which form the NGIB (Next Generation Industrial Biotechnology) concept. One adept is the gram-negative bacterium *Caldimonas thermodepolymerans* DSM 15344, which is capable of producing poly3-hydroxybutyrate (PHB) up to 87% w/w of CDM (20 g/L xylose). To enhance the biotechnological potential of this bacterium, genetic modification techniques have been employed, specifically in the form of deletions based on homologous recombination. In this work, we present a comparison of the biotechnological characteristics and stress robustness in three mutant strains of *C. thermodepolymerans* DSM15344 together with wild type itself. The genetically modified bacteria involved are: *C. thermodepolymerans ΔphaC* (derivative of DSM 15344 with deleted gene of PHA synthase IS481_08630); *C. thermodepolymerans AI01* (derivative of DSM 15344, deleted genes of restriction endonucleases: ΔIS481_08585, ΔIS481_14855, ΔIS4 81_14025); and *C. thermodepolymerans ΔphaZ* (derivative of *C. thermodepolymerans AI01*, deleted gene of PHA intracellular depolymerase IS481_07130). Under the guise of the biological consequences of gene deletions, we focused on the growth of bacteria on three different substrates – xylose, glucose and cellobiose (72 h at 50 °C) in terms of PHA production (except *C. thermodepolymerans ΔphaC*); stress robustness characterization of the mutants as compared to DSM 15344 wild type; and also comparison of molecular weights of synthesized PHB in *ΔphaZ* as compared to DSM 15344 wild type.

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UNLOCKING THE POTENTIAL OF YEAST EPS: OPTIMIZATION STRATEGIES FOR INDUSTRIAL APPLICATIONS

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Extracellular polymeric substances (EPS) have gained significant attention due to their structural diversity, biological activities, and broad applications in the food, pharmaceutical, and cosmetic industries. The production and composition of these substances protect yeasts from extreme environmental conditions, making EPS properties highly dependent on external factors. Yeast-derived EPS offer advantages over bacterial counterparts, such as higher yields and easier separation from the culture medium. Despite their great potential, the production and structural characterization of yeast EPS remain insufficiently explored.

This study aimed to identify the optimal carbon source for EPS production in carotenogenic yeasts and evaluate its effect on the synthesis of different EPS fractions, carotenoids, and lipids. Cultivations were performed under controlled conditions using various carbon sources, and the produced EPS, biomass, and their properties were analyzed using gravimetric, chromatographic, and microscopic methods.

The results revealed a strong correlation between the carbon source and EPS yield. The highest biomass increase (18.40 ± 1.62 g/L) was observed in *Cystofilobasidium macerans* cultivated on a sucrose-based medium, which also supported high EPS (7.17 ± 0.038 g/L) and lipid production (25.52 ± 0.17 %). These findings indicate that medium composition significantly influences both the quantity and composition of yeast EPS, highlighting the potential for targeted optimization.

This study emphasizes the importance of selecting appropriate carbon sources to enhance EPS synthesis and overall biomass production in carotenogenic yeasts. Furthermore, optimizing both cultivation parameters and EPS isolation methods could significantly improve their industrial applicability, making yeast EPS a promising alternative to bacterial polysaccharides.

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COMPARATIVE METHYLATION ANALYSIS OF *CALDIMONAS THERMODEPOLYMERANS* USING THIRD-GENERATION SEQUENCING

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DNA methylation in the bacterial genome plays an important role in epigenetic modification, which affects gene expression, regulation and environmental adaptation, etc. In this study, we conducted a comparative analysis of methylation patterns in the Gram-Negative bacteria *Caldimonas thermopolymerans* DSM 15344^T. The type strain was initially isolated from activated sludge in Germany and then deposited in Leibniz Institute DSMZ in Germany (CT-DSMZ) and later in the Czech Collection of Microorganisms in Czechia (CT-CCM). Our aim was to assess whether a change in cultivation conditions and phenotype characteristics of the cultures deposited in various public collections coincides with methylation patterns. We used Oxford Nanopore Technology (ONT) sequencing with R10.4.1 flow cells and V14 chemistry for more accurate analysis. Despite being the same strain, we observed a significant difference in methylation counts between these two samples. The sample CT-CCM showed 7,350 6mA modifications, 2,764 5mC modifications, and 732 4mC modifications, while the sample CT-DSMZ showed slightly lower modification counts, with 6,884 6mA, 2,681 5mC, and 643 4mC modifications. We also analysed the distribution of methylation across different genomic annotation features, such as coding sequences (CDS), rRNA, and tRNA regions. The analysis also revealed significant differences between the two samples. In the Coding sequences (CDS), CT-CCM showed 7,153 6mA modifications, 2,339 5mC modifications, and 708 4mC modifications, while CT-DSMZ showed slightly lower counts with 6,680 6mA, 2,290 5mC, and 620 4mC modifications. To enhance our detection of methylated bases, we employed the Pacific Biosciences (PacBio) Sequel IIe platform. We integrated the methylation data from both sequencing platforms while comparing the epigenomes of specific sample cultivation. The differences in methylation levels between these two cultures suggest the role of cultivation conditions like temperature and nutrient availability that may lead to unique epigenetic changes. Given the role played by methylation in gene regulation, our finding contributes to knowledge of the potential impact of cultivation conditions on bacterial physiology. Our research will help in enhancing our understanding of bacterial epigenetics and how the DNA methylation landscape is affected by the cultivation environment.

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TECHNOLOGY FOR ENVIRONMENTAL PROTECTION

LECTURES

KUTNÁ HORA, RISK ELEMENTS AND SHREDDED CARBOARD

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ČZU in Prague, Prague, The Czech republic
**at the time of creation*

The town of Kutná Hora (KH) and rural surroundings represent a locality significantly polluted with risk elements (RE) due to smelting and mining activities. These activities go back to the second half of the 13th century, and by the beginning of the 14th century KH had grown into one of the largest mining towns in Europe. In the first half of the 14th century 90% of annual silver production came from mining in KH.

Today, the unconfined deposits of slag and mining wastes still threaten the wider surrounding environment due to airborne deposition of small risk element-bearing particulates, and soils that are loaded with excessive amounts of As, Cd, Pb and Zn. These elements have potential to enter the food chain via soil/plant transfer and plant accumulation mechanisms. These facts were observed during the study of soil pollution in a gardening community and during the analysis of collected fruits and vegetables.

Susceptibility for contamination as well as mechanisms of leaching of selected risk elements were studied using batch and continuous leaching experiments. The influence of different types of low molecular mass organic acids (LMMOA) on release and transportation of these elements was evidenced. It is known that rhizosphere soil differs considerably from bulk soil, due to chemical reactions driven by LMMOA - the dynamic part of soil organic matter. Moreover, due to the great potential of LMMOA to form soluble complexes with various metals/metalloids, there is a demand for LMMOA isolation and application in some non-toxicity related soil remediation situations. Due to their alkaline properties caused by high content of calcium carbonates, and their significant anionic surface area for cation exchange, shredded carboard can serve as an effective sorption medium for risk elements released in this way.

Our study aimed to analyse different leaching solutions, with emphasis on LMMOA, for content of As, Cd, and Pb after passing through columns of contaminated soil with/without a shredded cardboard layer. We suggested the that the shredded carboard, probably even recycled paper, could be applied as an effective filter to remove risk elements from the extract solution following soil washing.

TRIBO-SORTING OF GRANULAR PLASTIC WASTE

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Although many separation/sorting techniques for plastic waste are known, they all have significant drawbacks, so none can be used universally. Our research focuses on improving the efficiency of a triboelectric sorting of plastics, a method that has the potential to become an important link in the recycling chain for many reasons, such as the low cost, no use of solvents and surfactants, possible separation of black materials, etc.

Triboelectric separation uses the tribocharging of shredded waste: different plastic materials obtain a different electrostatic charge by frictional contact with a suitable counter-material. Charged plastic pieces are then separated during a free fall between electrodes in the electrostatic separator. The choice of counter-material is the most challenging task in designing a triboelectric separator, as it plays a crucial role in controlling the charge of individual plastic pieces. Our self-constructed charging devices allow for: (i) contact by rotational or vibrational motion, (ii) contact by fluidization, and (iii) charging by corona discharge. The average charge in a sample is measured using a Faraday pail and an electrometer.

We have focused on improving electrostatic separation by finding suitable counter-materials to effectively separate multi-component plastic mixtures by separating one material per cycle and then recharging the remaining mixture with different counter-materials during the next cycle. The corona discharge has been attempted to shorten the time needed to achieve the saturation charge on individual plastic waste particles. The choice of the counter-material and charging method can control the magnitude and, in some cases, even the polarity. We demonstrate various tribo-sorting case studies of 3-component mixtures.

NITRIFICATION INHIBITORS ON THE SURFACE OF GRANULAR FERTILIZERS

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Nitrogen (N) is a keyplant nutrient and is usually one of the most limit ingelements for cropproduction. Farmers must carefully consider the use of nitrogen fertilizers. It is estimated that more than 50% of the applied nitrogen is not used due the to various biological, physical and chemical processes. These include leaching of nitrates (NO_3^-) into water and emission of ammonia (NH_3) and nitrogen oxides (N_2O, NO_x) into the atmosphere. The relatively low efficiency of nitrogen use leads to significant environmental impacts. The use of nitrification inhibitors helps to preserve possible forms of nitrogen for a longer period in the root systems of crops, reduces nitrogen loss and permits more efficient utilization. Nitrification inhibitors have the potential to reduce emissions of NH_3 or N_2O to the atmosphere and to reduce the amount of $NO_3{}^-$ leached from the surface layers of the soil [1,2].

It is known that 4-hydroxycinnamic acid methyl ester (HAME) is a relatively good natural nitrification inhibitor. Analogues of 4-hydroxycinnamic acid methyl ester were prepared for testing in the laboratory research of VUCHT j.s.c.. HAME is found in the root exudates of the tropical grass Brachiariahumidicola, where two phenylpropanoids, methyl-p-

coumarate (HAME) and methylferulate, were identified as responsible for the activity of a biological nitrification inhibitor in the root tissues of this grass[3].
In the laboratories of VUCHT j.s.c. were studied and tested the properties of the nitrification inhibitor of nitrogen fertilizers in the form of guanidine polymers (guanidine hydrochloride with diamine compounds) and a copolymer of the polymer guanidine hydrochloride with 1,2 diaminopropane and ε-caprolactone were investigated. The prepared polymers and copolymers were applied to the surface of granular nitrogen fertilizers[4].
Both nitrification inhibitors on the surface of granular fertilizers were tested in small-plot field experiments on agricultural crops such as winter wheat, winter rapeseed and seed corn, as well as in soil pot tests.
REFERENCES

1. Ing. Zdenko Tokár, VUCHT a.s. SLOWUREA – zvýšenie efektivity močovinových hnojív 2021 https://www.mojehnojiva.cz/aktuality/slowurea-zvysenie-efektivity-mocovinovych-hnojiv

2. Ducsay L &Varényiová M (2020) Aplikácie hnojív s inhibíciou nitrifikácie, Naše pole, https://nasepole.sk/aplikacia-hnojiv-s-inhibiciou-nitrifikacie

3. Gopalakrishnan S, Subbarao GV, Nakahara K, Yoshihashi T, Ito O,Maeda I, Ono H, Yoshida M (2007) Nitrification Inhibitors from the roottissues of Brachiariahumidicola, a tropicalgrass. J AgricFoodChem 55:1385–1388.https://pubs.acs.org/doi/10.1021/jf062593o

4. Aleksandrovich, Stel'makh&Grigor'eva, M. &Garkusheva, N. &Lebedeva, S. &Ochirov, O. &Mognonov, D. & Zhamsaranova, S. & Batoev, Valeriy. (2021). Studies of new biocidal polyguanidines: antibacterialaction and toxicity. Polymer Bulletin. 78. 10.1007/s00289-020-03197-1.
https://www.researchgate.net/publication/340879994_Studies_of_new_biocidal_polyguanidines_antibacterial_action_and_toxicity

COMPARISON OF CATALYTIC PERFORMANCES OF PT/TI$_X$CE$_Y$O$_N$ CATALYSTS AND TRANSITION METAL (TI, CU, FE) AND LANTHANIDE (CE) - BASED OXIDE CATALYSTS FOR DICHLOROMETHANE OXIDATION

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Dichloromethane is classified as a Class 2A compounds , a probable human carcinogen. Dichloromethane (DCM) is one of many substances classified as a chlorinated volatile organic compound (CVOC) that definitively pose a risks to a human health and the environment [1,2]. Catalytic oxidation is one of the most technologically and economically acceptable technologies for the CVOCs reduction due to its simplicity and high efficiency. In recent years, efforts have been made to develop a highly active, selective and durable catalyst for CVOCs oxidation and to reduce the carbon footprint [3,4].

The aim of this work is to compare the catalytic performance of two sets of granulated catalysts prepared by co-precipitation in dichloromethane oxidation. The first set of catalysts contains impregnated Pt on various TiO_2-CeO_2, the second set of catalysts is composed of a mixture of TiO_2, CeO_2, CuO and Fe_2O_3. The prepared catalysts were tested in dichloromethane oxidation using light-off tests in temperature range of 100-500°C in a flow reactor connected to online FTIR.

The catalysts activity and HCl selectivity is comparable for both prepared catalyst sets. The best Pt/TiO_2 from the first set shows T_{95} 318 °C with HCl yiled 87 % and the best TiO_2-Fe_2O_3 from the second set shows T_{95} 327 °C with HCl yield 91 %. But, the CO_2 selectivity and the amount of detected unwanted by-products (CH_2O, CO) differ. The Pt-impregnated catalysts exhibit lower amounts of detected by-products and higher CO_2 selectivity compared to the second catalyst set. The reason of this is better reducibility of Pt-impregnated catalysts.

References

[1] Fan, M.J., et al., Enhanced catalytic oxidation of dichloromethane by a surfactant-modified CeO_2@TiO_2 core-shell nanostructured catalyst. Journal of Rare Earths, 2023. 41(7): p. 1031-1041.

[2] Wang, P., et al., Progress in Degradation of Volatile Organic Compounds by Catalytic Oxidation: a Review Based on the Kinds of Active Components of Catalysts. Water Air and Soil Pollution, 2024. 235(1).

[3] Huang, H.B., et al., Low temperature catalytic oxidation of volatile organic compounds: a review. Catalysis Science & Technology, 2015. 5(5): p. 2649-2669.

[4] Pitkäaho, S., et al., Catalytic Oxidation of Dichloromethane and Perchloroethylene: Laboratory and Industrial Scale Studies. Topics in Catalysis, 2011. 54(16-18): p. 1257-1265.

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MICROWAVE TRANSFORMATION OF WASTE HDPE INTO HIGH-VALUE PRODUCTS

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Global plastic production has increased from 2 million tons in the 1970s to 383 million tons in 2020, with this trend further intensifying after the COVID-19 pandemic. Although HDPE is widely used in households and industry, the global recycling rate remains low—only 20% of plastics are recycled, while 50% end up in landfills and 30% are incinerated.

An alternative to plastic recycling is microwave processing, which transforms and valorizes polymer waste into valuable gases or condensates and/or waxes. The microwave method utilizes dielectric heating, which rapidly heats and breaks down plastic molecules. A challenge is that some plastics, such as HDPE, are transparent to microwaves, requiring the addition of a microwave absorber, such as activated carbon (AC) or silicon carbide (SiC), to ensure microwave absorption in the plastic mixture.

In this study, HDPE was processed using activated carbon (with a carbon content > 99%) and silicon carbide under mild conditions (heating at 10°C/min to 260°C, 30 minutes, max. 500 W). The entire decomposition process took place in an oxidative atmosphere of ambient air, where oxygen constitutes 21 vol%, nitrogen 78 vol% and other gases 1 vol%. The result was the conversion of HDPE into gas (AC – 8.9 wt%, SiC – 9.5 wt%), wax (AC – 24.2 wt%, SiC – 17.0 wt%) and a carbonaceous solid residue (AC – 66.9 wt%, SiC – 73.5 wt%). The gaseous fraction contained hydrogen (AC - 6.72 mmol H_2/g_{HDPE}, SiC – 0.4 mmol H_2/g_{HDPE}), carbon monoxide, carbon dioxide, methane, and C_2–C_5 hydrocarbons. No condensate was produced, but solid waxes were obtained. In the case of AC, the waxes primarily consisted of n-alkenes (81.2 wt%), followed by 1-alkenes (11.5 wt%), with minor amounts of aromatic (0.9 wt%) and polycyclic aromatic hydrocarbons (4 wt%). For SiC, the waxes contained 1-alkanes (31.7 wt%), n-alkanes (29 wt%), dienes (16.2 wt%), as well as alcohols (12.3 wt%) and aldehydes (8.1 wt%). Carbon chains longer than C_{30+} could not be accurately evaluated. The waxes contained C_{30+} chain lengths only in minimal amounts of AC-W_{30+} (2.4 wt.%) and SiC-W_{30+} (2.7 wt.%).

The study confirms that microwave processing of HDPE with carbon-based absorbers enables hydrogen production under mild conditions and the recovery of valuable raw materials. Further research is currently underway to optimize microwave processing parameters with the aim of increasing hydrogen yield.

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TECHNOLOGY FOR ENVIRONMENTAL PROTECTION

POSTERS

TESTING THE ECOTOXICITY OF CIGARETTE BUTTS AND THEIR IMPACT ON THE ENVIRONMENT

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Cigarette butts are one of the few wastes that are systematically addressed. However, the scientific community has been dealing with their issue for several years, mainly due to their potential toxicity and high annual volume production.

The impact of chemical substances on the environment is assessed by ecotoxicological tests. They are classified into many different groups according to their nature. The most common classification parameters are the duration of the test (acute, sub chronic and chronic), the environment in which it is carried out (terrestrial or aquatic), and the organism tested.

In this work, three toxicity tests were performed in cooperation with VÚOS a.s., Rybitví according to OECD methodologies: (i) acute toxicity test corresponding to OECD Guideline No. 201 on the freshwater crustacean *Daphnia magna* (Fig. 1 a), (ii) sub chronic toxicity test No. 202 on the freshwater alga *Desmodesmus subspicatus* (Fig. 1 b) and (iii) activated sludge respiration inhibition test No. 209.

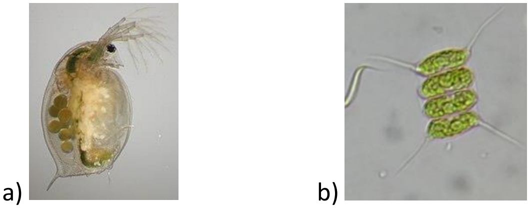

Figure 1 Organisms used *Daphnia magna* (a); *Desmodesmus subspicatus* (b)

The toxicity of the extract from cigarette butts, which was prepared by mixing the required number of cigarette butts in drinking water for 24 hours, was tested on the mentioned organisms. The mortality of the organisms was evaluated using the ToxRatPro Version 3.3.0 program and the values of the lethal concentrations EC50 and ErC50 were obtained. For *Daphnia magna*, the EC50 was found for the 24-hour test = 0.81 cigarette butts per litre of dilution water and for the 48-hour test = 0.39 cigarette butts. For *Desmodesmus subspicatus*, the toxicity was significantly lower, for the 72-hour test ErC50 = 23.03 cigarette butts per litre of dilution water was found. In the activated sludge test, no deviation from the control group was found even for the highest concentration of extract used (16 cigarette butts per litre of dilution water).

According to the current legislation, cigarette butts cannot be included in the list of acutely ecotoxic substances.

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TECHNICAL SOLUTION FOR THE DISPOSAL OF LIQUID HAZARDOUS WASTE USING THERMAL PLASMA

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As a result of human activities, a large amount of waste is produced, including waste that is hazardous to the environment and humans. The disposal of these wastes is generally very challenging, and it is essential to ensure that the process does not harm the environment. Plasma gasification appears to be a suitable technology for waste disposal. This technology uses the effect of very high temperatures (around 1200 °C), which leads to the conversion of organic materials into syngas, containing hydrogen (H2) and carbon dioxide (CO2), while inorganic components are melted into inert, non-leachable slag. The syngas can be used in industrial processes, or hydrogen can be separated from it as a potential energy source. The disadvantage of this technology is its high energy demand, making it necessary to combine it with renewable energy sources to maximize its ecological and economic efficiency.

This research focused on the design and development of a system for the injection of liquid substances containing persistent organic pollutants (POPs) into the plasma gasification technology. A system was designed and constructed that can effectively dose liquids, such as transformer oil or pyrolysis liquids, into the already existing plasma gasifier technology for solid wastes and biomass. This process can significantly contribute to the efficient processing of specific waste substances that cannot be easily disposed of by traditional methods, while minimizing the negative impact on the environment.

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AUTOMATED CALCULATION OF THE WASTEWATER MATERIAL BALANCE IN THE WASTEWATER TREATMENT PROCESS

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Nowadays, environmental requirements are often increasing and becoming more stringent, so an accurate calculation of the material balance of wastewater in the management of purification systems is necessary to know what needs to be changed in a particular process. This work presents a program for calculating the material balance of wastewater considering such parameters as chemical oxygen demand (COD), biochemical oxygen demand (BOD), fluorine (F) or, for example, adsorbable organic halides (AOX). It is known that the water purification process consists of several stages. Processes occurring at each stage of purification can be modeled, for this it is only necessary to know the quantities and qualities of incoming or outgoing streams. The developed model allows us to evaluate not only theoretical purification indicators but also consider the actual cleaning efficiency after each stage of water purification, which brings the calculation closer to practice and allows us to compare real and theoretically possible data. That is, the main feature of the program is aimed at the ability to compare theoretical and real purification efficiency. The program allows us to analyze wastewater flows at various stages of treatment in the system, determining quantitative and qualitative changes in parameters. The model can be useful for specialists in the field of water treatment and ecology and can also be used in industrial enterprises to assess the efficiency of existing treatment facilities and optimize their operation. The program allows us to predict the degree of water purification and, thus, help make more informed decisions when managing water resources. Its use helps reduce environmental risks and improve the efficiency of wastewater management.

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