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TRANSFORMÁCIA ENERGIE DO CHEMIKÁLIÍ A PALÍV POWER-TO-X-TECHNOLOGY

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V prednáške sa zameriam na pochopenie kľúčového postavenia petrochemického priemyslu, pri transformácii energetiky formou integrácie obnoviteľných alebo nízko-uhlíkových alternatív. Kľúčom k dekarbonizácii je Power-to-X-Petrochemical Technology.

Prvým krokom je zachytávanie oxidu uhličitého. Najčastejšie sa spomína v spojení s potenciálnym riešením krízy globálneho otepľovania. Podľa Medzinárodnej energetickej agentúry (IEA) v roku 2023 emisie oxidu uhličitého predstavovali 36,8 megaton. S väčšinou zachyteného uhlíka sa však v súčasnosti nakladá ako s odpadom. Zachytené množstvo sa likviduje, a nepoužíva zmysluplným spôsobom. Napriek tomu, z hľadiska trvalo udržateľného rozvoja, zhodnocovanie oxidu uhličitého môže patriť medzi veľmi príťažlivé východiskové suroviny pre chemické technológie. Avšak, ponúkne ekonomický potenciál len v tom prípade, keď sa táto nízko-uhlíková zlúčenina, ako východisková surovina, konvertuje na lacnejšie chemikálie a palivá v porovnaní s ich súčasnými cenami.

Vďaka tomu, pre tie krajiny, ktoré sa snažia dosiahnuť nulové uhlíkové emisie sa vodík stane kľúčovou súčasťou dekarbonizačného reťazca v chemicko-technologických uzloch. Na dekarbonizáciu sa doposiaľ používal hlavne elektrický prúd. Jasným príkladom toho v súčasnosti je rastúci nástup elektromobility. Aj keď existuje veľa ďalších príkladov, ako možno elektrinu použiť na dekarbonizáciu, nie je to použiteľné v každom sektore alebo priemyselnom odvetví. Obrovské množstvá vodíka sa už v súčasnosti bezpečne používajú pri spracovaní v rafinériach ropy, v petrochémii, pri výrobe umelých hnojív i v ďalších priemyselných odvetviach. Novo navrhované vodíkové centrá v technologických uzloch budú sofistikovaným a zložitým ekosystémom, ktorý pokryje celý dodávateľský reťazec.

Od konca minulého storočia badať v chemickej technológii zvýšený záujem o chémiu C1. Jedná sa hlavne o štyri chemikálie, z ktorých majú významné priemyselné využitie: metán, oxid uhoľnatý, oxid uhličitý a metanol. Oxid uhličitý je vo veľkom zriedení vo vzduchu nevyhnutným komponentom pre fotosyntézu rastlín a drevín. V pomerne vysokých koncentráciách je zložkou zemného plynu z niektorých ložísk. Nachádza sa však predovšetkým v plynných splodinách a exhalátoch z viacerých chemických procesov. Najvýraznejší podiel prichádza zo spaľovania tuhých, kvapalných a plynných fosílnych palív. Napriek obrovskému celosvetovému vzrastu uhlíkových emisií na úroveň 36 800 miliónov ton oxidu uhličitého, patrí zatiaľ oxid uhličitý k menej chemicky zhodnocovaným surovinám. Jednou zo základných príčin je skutočnosť, že spolu s vodou je termodynamicky konečným produktom mnohých chemických procesov. Preto k použitiu oxidu uhličitého ako zdroja uhlíka si vyžaduje výrazný energetický vklad (vodík, elektródové procesy, karbanióny a pod.).

Napriek tomu, oxid uhličitý patrí medzi relatívne významné priemyselné suroviny, ktoré sa v minulosti aj v súčasnosti finalizujú v stovkách miliónov ton. Pri pohľade cez anorganickú optikou výrobkov, viac ako polovica tohto množstva sa používa vo forme chladiacich médií. Štvrtina sa používa na prípravu sýtených nápojov. Kvapalný oxid uhličitý sa používa na výrobu tuhého oxidu známeho ako suchý ľad, ktorý môžeme skladovať pri izbovej teplote. Nízka teplota sublimácie (-78,5 °C) robí suchý ľad efektívnym a často používaným chladiacim médiom. Oxid uhličitý sa používa ako hnací plyn (propelent) v sprejoch a na naplnenie záchranných člnov a viest. Oxid uhličitý je perfektnou náhradou 1,2-dibrómmetánu, brómmetánu alebo fosfánu pri úschove obilia v poľnohospodárskych silách. Prvý je v súčasnosti považovaný za karcinogén, druhý vo vrchných vrstvách atmosféry rozkladá ozón a tretí je pre človeka vysokorizikovou zlúčeninou. Hmyz v obilných silách nemá šancu prežiť v atmosfére oxidu uhličitého.

Cez optiku petrochémie, vidíme oxid uhličitý (skvapalnený, plynnej forme, vo vodnom roztoku ako kyselina uhličitá alebo suchý ľad) nachádzajúci použitie nielen ako chladiace činidlo, ale aj ako rozpúšťadlo (superkritickom stave), v zlievarenstve, najmä však ako surovina, pri výrobe močoviny, kyseliny salicylovej a jej derivátov, etylénkarbonátu, propylénkarbonátu, a uhličitanu sodného (Solvayov spôsob z NaCl, Leblankov zo sadrovca), draselného a amónneho.

Výroba močoviny je úzko spojená s výrobou amoniaku. Okrem amoniaku sa využíva aj oxid uhličitý, vznikajúci pri príprave syntézneho plynu. Močovina sa v Českej republike do roku 2012 vyrábala v Unipetrole Litvínov. Na Slovensku sa výrobí ročne 390 000 ton močoviny v spoločnosti Duslo Šaľa (v rokoch 2022-2026 s 3,1% rastom), ktorá je súčasťou skupiny Agrofert. Svetová produkcia močoviny je na úrovni 180 miliónov ton/ročne (2021). Orlen Unipetrol pokračuje v modernizácii výroby amoniaku (2023), ktorá prinesie zlepšenie produkcie na 180 000 ton/ročne a zníženie emisií oxidu uhličitého.

Kyselina salicylová je významným medziproduktom nielen pri výrobe liečiv (kyseliny acetylsalicylovej, pod obchodnými značkami Aspirin, Acylpirin, Anopyrin, atď.), ale aj C-alkylsalicylátov, ktoré sú prísadami do mazacích olejov. Vyrába sa Kolbeho-Schmitovou syntézou z bezvodného fenolátu, resp. alkylfenolátu sodného a oxidu uhličitého. Svetová produkcia kyseliny salicylovej dosahuje 90 000 ton/ročne (2015). V roku 2022 sa vyrobilo 40 000 ton Aspirinu ročne.

Uhlíková stopa nám celosvetovo neustále rastie. Stále je dlhšia, širšia a hlbšia. Najväčšou mierou sa na emisiách oxidu uhličitého podieľa výroba elektriny a tepla. Nasleduje doprava, priemysel, domácnosti, poľnohospodárstvo, komerčné a verejné služby i malé priemyselné odvetvia. V chemickej technológii je to predovšetkým výroba etylénoxidu, amoniaku, čistenie zemného plynu, a fermentačné procesy. Ďalšími priemyselnými zdrojmi sú oceliarstvo a cementárne. Najviac oxidu uhličitého však uniká do atmosféry, ako som predtým uviedol, spaľovaním fosílnych palív v elektrárňach a teplárňach.

V tomto ohľade moja prezentácia bude zahŕňať pomerne širokú škálu nových, moderných procesov. Uvidíme, že dosiahnutie ekologickej premeny oxidu uhličitého na široké spektrum želaných produktov je finančne (ekonomicky) veľmi náročné. Častokrát sú to procesy s nízkym TRL, od jedna do sedem. Nezameriavam sa len na konkrétnu reakciu alebo spôsob výroby. V prednáške spájam skôr teoretické (termodynamické, kinetické, reaktorové, katalytické) a technológicke aspekty. Snažím sa poskytnúť oveľa hlbší obraz prezentovanej témy. Diskutujem o mnohých spôsoboch a procesoch, akými sú termochemická, elektrochemická, fotochemická, fotoelektrochemická, biochemická a nukleárnou energiou podporovaná transformácia.
Na základe súčasného stavu zhodnocovania oxidu uhličitého, ako aj existujúcich alternatív a stimulujúcich vyhliadok, zohľadňujem skutočnosti, ktoré obmedzujú používanie takýchto technológií. Osobitný dôraz kladiem na optimalizáciu reakčných podmienok, vývoj a aplikáciu nových katalyzátorov umožňujúcich čo najlepšiu výrobu cenných a ekologicky netoxických zlúčenín z oxidu uhličitého.

Na jednej strane v prezentácii poukážem na prijaté výzvy súvisiace s aplikáciou zhodnocovania oxidu uhličitého. Na strane druhej konfrontujem možnosti stotožnenia sa s nimi v priemyselnom meradle. Veľkú dôležitosť pripisujem aj nasmerovaniu ďalšieho vedeckého výskumu v tejto oblasti. Citlivo hodnotím perspektívy moderných vodíkových technológií. Poukážem na rastúci počet publikovaných prác na túto tému. Ale len obmedzený počet prác, ponúka reálne dostupnú petrochemickú cestu. Verím, že moja prezentácia bude cenným doplnkom mnohým výskumníkom. Rovnako pomôže aj priemyselne vyspelým technologickým hráčom, majúcich záujem investovať a rozvíjať nové, sľubne sa rozvíjajúce procesy a technológie.

Želajme si, aby sme čo najskôr nabrali odvahu vystúpiť z montážnych hál miliónových produkcií automobilov, podľa nemeckých, francúzskych, kórejských, švédskych licencií. Rovnako autobatérií podľa čínskych licencií. Čo najskôr začnime presadzovať originálne výsledky vlastného vedeckého výskumu, vývoja a inovácií. Stojíme na začiatku petrochemickej cesty Power-to-X-Technology. Viem, že nestačí o takejto výzve len hovoriť a následne ju prijať. Oveľa dôležitejšie bude sa s výzvou stotožniť. Stále rezonuje otázka, kde je potrebné u nás hľadať, respektíve odkiaľ zoberieme, také obrovské kvantá nadbytočnej, pritom lacnej a čistej energie

Ďalekosiahlou alternatívou ku všetkým iným energetickým zdrojom je na Slovensku a v Českej republike jadrová energia. Už teraz je zrejmé, že dosiahnutie nulových emisií oxidu uhličitého do roku 2050 nebude možné ani u nás bez určitého podielu jadrovej energie. Toto moje jednoznačné konštatovanie nevyplýva len z mojich kníh, ale podporuje ho aj deklarácia prijatá koncom minulého roka viac než 20. krajinami na klimatickej konferencii Organizácie Spojených národov COP28 v Dubaji. Účastníci v decembri 2023 podporili až trojnásobné navýšenie svetovej kapacity jadrovej energie do roku 2050. V porovnaní s úrovňou z roku 2020. Dubajskú deklaráciu podpísali aj Slovensko a Česká republika. Jadrová energetika má podľa deklarácie dôležitú úlohu v úsilí dosiahnuť do roku 2050

uhlíkovú neutralitu. To znamená, buď dosiahnutie nulových emisií oxidu uhličitého, alebo ich vyváženie opatreniami, ktorých účinok bude ekvivalentný.
Už v súčasnosti v Európskej Únii patrí Slovensko a Česká republika spolu s Francúzskom k významným hráčom pri výrobe elektrickej energie z nefosílnych palív. Slovensko vyrobilo v roku 2019: 54% elektrickej energie v jadrových elektrárňach. K ním pribudol v roku 2023 tretí 500 MW blok v Mochovciach. Rozostavaný je ešte štvrtý blok. 16% elektriny vyrobilo Slovensko vo vodných elektrárňach. 6% v elektrárňach na biomasu. Česká republika už niekoľko rokov patrí medzi významných európskych lídrov v oblasti výskumu jadrovej energetiky (ÚJV Řež). HeFASTo je originálny koncept malého modulárneho reaktora (SMR), ktorý je založený na technológii plynom (héliom) chladeného rýchleho reaktora. Energywell je patentovaný SMR, ktorý využíva technológiu na báze roztavenej soli. Oba jadrové projekty sú podľa Českých energetických závodov v pokročilom štádiu výskumu. Cieľom je výroba vodíka v technologických uzloch pre jednotlivé priemyselné odvetvia.

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„Green“ Hydrogen Production by Means of Water Electrolysis

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As a „green“ is marked hydrogen produced with no, or very low carbon dioxide emissions. Among the technologies of green hydrogen production, water electrolysis clearly dominates. Most of the industrial technologies planned to be introduced in order to achieve the economy decarbonisation and at the same time, diversification of the energy sources relies on the green hydrogen. Therefore, water electrolysis comes into the centre of interest of not only the research establishments, but also of the related industry.

Despite water electrolysis represents oldest technology of the industrial scale hydrogen production, its share on the global hydrogen production represents nowadays only approximately 4 %. It is thus clear, that current water electrolysis technology needs significant improvements in order to become acceptable alternative to the traditional fossil fuels technologies.

Historically, alkaline water electrolysis utilizing concentrated KOH as a liquid electrolyte was developed more or less as the exclusive approach to this process. With an increasing pressure on the process efficiency and flexibility caused by its connection to the renewable energy sources, required innovation led to alternative approaches. Two directions were developed intensively. They include at first development of acidic version other process based on utilization of the perfluorinated sulfonated acids as a solid polymer electrolyte (PEM water electrolysis). This process is characterized by very high intensity and flexibility when compared to the traditional alkaline process. Negative aspect represent its material demands. As a second alternative, high temperature process based on ceramic electrolytes is developed under the name of solid oxides electrolysis cell (SOEC). It is characterized by high process intensity and efficiency, unfortunately at the expense of flexibility. Recently, main effort is to develop new generation of the water electrolysis process combining advantages of PEM and alkaline process in one, namely alkaline membrane water electrolysis.

It is a target of this presentation to provide basic overview of the state of the art in the field of green hydrogen production by the water electrolysis and of the directions of development expected in the nearest future.

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Hydrogen Strategy of the Czech Republic

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During the development of updated national hydrogen strategy, we recognised that a singular, linear approach to strategy development was unable to bring us to required outcomes. It was a reason why we divided the strategy into three distinct phases, each with unique ambitions, objectives, hydrogen pricing structures, and implementation tools.

The initial phase, named "Local Islands," focuses on local hydrogen production from renewable sources. Although this approach may be costly—estimated approximately with some subsidies over 8 EUR per kg of hydrogen—it remains a necessary step, particularly for meeting mandatory targets in mobility and the chemical industry. Given the complexities of importing renewable hydrogen, primarily due to our geographic constraints, this approach is imperative.

To mitigate costs of the renewable hydrogen produced in the Czech Republic, we aim to source hydrogen from regions with surplus renewable resources as early as possible. It means to import hydrogen from regions such as Southern and Northern Europe, North Africa, the Near East, Ukraine, Canada, or the USA. Transitioning our gas transport network to accommodate hydrogen is the primary objective of the second phase, known as "Global Bridges." Leveraging the robustness of our existing natural gas infrastructure, we can repurpose select pipelines without the need for extensive construction. Notably, the Czech German Hydrogen Interconnector and the Central European Hydrogen Corridor will play pivotal roles in importing renewable hydrogen from neighbouring regions. We anticipate that imported hydrogen prices will decrease to around 4 EUR per kg.

While importing renewable hydrogen may lower costs, it also heightens our energy dependency on other countries. Therefore, our long-term strategy aims to diversify hydrogen imports while investing in domestic resources. Given our limited renewable potential, we must explore alternative technologies, such as high-temperature electrolysis utilising nuclear power and geothermal energy. These innovations, anticipated by the phase "New Technologies" around 2045, aim to reduce hydrogen production costs to approximately 2 EUR per kg, thereby facilitating widespread adoption across various sectors.

Our objectives, outlined by the Renewable Energy Directive, include replacing 40,000 t of grey hydrogen with renewable alternatives in transportation and chemical industries, alongside with establishing a network of hydrogen refuelling stations as outlined in AFIR. Achieving these goals requires installing from 300 to 400 MW of electrolysers and associated renewable resources as wind and solar farms. On the consumption side, we aspire to integrate hydrogen into heavy-duty road transport, bus services, and regional train networks.

4-Chinolónové liečivá a ich perspektíva

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4-Chinolóny sú heterocyklické systémy, ktoré majú vysokú termickú stabilitu. Pripravujú sa zvyčajne termickou cyklokondenzačnou reakciou pri teplotách okolo 250 °C alebo za použitia kyslej či bázickej katalýzy. Aj napriek tomu sa nachádzajú aj v prírode v živočíšnej i rastlinnej ríši. Ich substituované a/alebo kondenzované deriváty sa vyznačujú viacerými typmi biologickej aktivity, najmä však antibakteriálnou, protirakovinovou, v poslednej dobe dokonca aj antialzheimerickou a inými aktivitami. Z tohoto dôvodu sú to zlúčeniny, o ktoré je neustály záujem.

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-17-0513 a APVV-20-0213.

Materials engineering

Correlation of Plastic Deformation of Metastable Cu-Ag Metal-Matrix Composites

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As metal-matrix composites (MMCs), the materials are usually considered to contain soft matrix and hard particulates of various shapes as they can well serve numerous practical applications. From the viewpoint of understanding some detailed mechanisms, it is also interesting to study MMCs containing the soft matrix as well as the soft particulates. In this contribution, we refer to the plastic deformation of Cu–Ag MMCs produced by spark plasma sintering the Cu@Ag core-shell powders. Plastic deformation of such MMCs possesses a similar true stress–true strain dependence. This dependence can be phenomenologically described by the logarithmic dependence of the modified Ramsberg-Osgood law but surprisingly, also by quadratic functions. The parameters of these dependences are specified, quantified, and discussed with respect to those of pure Ag and Cu as well as to the values of a cast Cu–Ag alloy of comparable composition. Besides, the plastic deformation results in the prolongation of the particulates relative to the straining of the MMC, i.e., in the direction of tensile deformation and perpendicularly to the direction of compression. The aspect ratio of the particulates is related to the value of the strain, and it is shown that these values fit with a proposed model of sphere deformation.

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Waste by-products as a source for carbides preparation for advanced alloys

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Introduction

The pyrolysis of plastic materials is constantly increasing its attraction due to its potential as a promising method for processing polymeric waste materials, ultimately yielding hydrogen as a primary product. Concurrently, this process generates carbon-bearing structures as by-products, often comprising carbon nanotubes or nanospheres. However, the purity of these structures is frequently influenced by catalysts or the compositions of the input materials being processed. Nevertheless, the carbon by-product holds substantial interest, owing to its high specific surface area, promoting rapid reactions with metals forming carbides. These carbides present an economically viable yet highly competitive option as reinforcing particles for a range of advanced materials, including high-entropy alloys.

Methodology

The optimization of process parameters involved varying the metal-to-carbon atomic ratios of 1:1 and 1:2. Additionally, the impact of the presence of a Process Control Agent (PCA) and the total process duration was assessed using XRD and XRF analyses. The most favourable combination of parameters was utilized for preparing a composite material comprising 5, 10, and 15 wt.% of reinforcing carbide particles within the CoCrFeNiMn alloy matrix.

Results

Various types of Me-C carbides (where Me = Ti, Nb, W) were synthesized via mechanical alloying, employing pure metals and carbon waste by-products obtained from polypropylene pyrolysis. The optimization of carbide synthesis was achieved successfully, resulting in the formation of a sufficient volume fraction of carbides. Furthermore, annealing at a temperature of 1000 °C (corresponding to SPS compaction conditions) led to a further increase in carbide content. Different types of prepared carbides and their weight amounts had different impacts on the composite properties.

Conclusion

The optimal parameters for carbide formation were individually determined for each elemental type. Subsequently, the carbides synthesized under these optimized conditions were employed as reinforcing particles within the newly formed composite CoCrFeNiMn alloy.

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POWDER METALLURGY PREPARATION OF SILICIDE-ALUMINIDE COMPOSITES

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In current industry, cemented carbide is widely used as the tool material for many purposes, e.g. machining or drilling. However, its main components – tungsten and cobalt – are listed by European Commission as the critical raw materials with very high supply risk. Therefore, there is a research activity to substitute these elements. It can be potentially done by three ways – substitution of tungsten by other carbide-forming element, substitution of cobalt binder or the design of a material without these elements. The latter approach was selected in this work, which aims at the solution based on combination of two intermetallics – iron silicide and suitable transition metal aluminide. Optimization of the preparation of the composite by powder metallurgy combining mechanical alloying and spark plasma sintering is presented in this work, together with basic characterization of the prepared composite.

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High-Temperature Oxidation of Refractory High-Entropy Alloys Prepared by Powder Metallurgy Methods

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Introduction

Refractory high-entropy alloys (RHEAs) are advanced materials whose structure is formed by solid solutions of 5 or more high-melting elements. A typical representative is the MoNbTaVW alloy, which is characterized not only by excellent heat resistance but also by rapid oxidation at elevated temperatures. This is mainly due to the content of Mo and V, whose oxides are not well stable at high temperatures.

Methods

To improve the high-temperature oxidation resistance of the reference MoNbTaVW alloy, the Mo and V were substituted by elements with better oxidation properties (Al, Ti, Cr, Ni). Powder metallurgy methods, comprising mechanical alloying and spark plasma sintering, were used to prepare the alloys. The microstructure and phase composition of these alloys were observed, and their mechanical properties were measured. Furthermore, the high-temperature oxidation and mechanical properties at high temperatures were determined.

Results

The well-refined and homogeneous microstructure was investigated using scanning electron microscopy, and the phase composition was determined using XRD analysis. As a result, the alloys achieved good mechanical and tribological properties, although a significant reduction in plasticity was observed compared to the reference alloy. In terms of resistance to high-temperature oxidation, it was found that alloying by Al and Ti yielded better oxidation properties than alloying by Cr and Ni.

Conclusion

Improved high-temperature oxidation resistance was observed for the prepared materials compared to the MoNbTaVW alloy. However, at the same time, the substitution of Mo and V decreased the mechanical properties due to the increase in the brittleness of these materials.

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Ignition-Resistant Magnesium Alloys Containing Calcium and Yttrium

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Introduction

Due to its low density and high strength-to-weight ratio, magnesium and its alloys are materials used in the automotive and aerospace industries. While some magnesium alloys achieve elevated ignition temperatures, they often rely on costly alloying elements. The main idea of this study is to find a simple way to experimentally test a large number of materials with different chemical compositions in terms of ignition temperature while developing ignition-resistant Mg-Y-Ca-Al-Zn alloys with reduced expensive component content.

Methods

Two groups of materials were prepared with the first one being prepared by hot extrusion and the second one being prepared from mixed powders with subsequent compacting by spark plasma sintering (SPS). The microstructures of the materials were examined by optical and electron microscopy and X-ray diffraction. The influence of materials processing on the ignition resistance was investigated using a standard test in which the sample was heated under constant airflow in the furnace. Furthermore, the oxide layers formed on the surface at elevated temperatures were examined.

Results

The ignition resistance tests revealed consistent values across all systems, irrespective of the processing methods. These materials demonstrated outstanding ignition resistance, requiring temperatures exceeding 1100 °C to ignite. Additionally, the formed oxide layers consisted of a mixture of calcium and yttrium oxides in both cases.

Conclusion

The results of this study showed comparable ignition resistance for materials prepared by hot extrusion and spark plasma sintering, finding a simple way that could enable us to experimentally assess a wide range of materials with varying chemical compositions regarding ignition temperature.

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THE TIN PEST ACCELERATION BY MEANS OF THE PINK SALT

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Tin pest is degradation mechanism of tin and tin rich alloys that is based on change of modification from white tin to grey tin at temperatures lower than 13 °C. It is well known that the process is influenced by temperature, inoculation, and composition of the alloy, although the effect of individual components is not clear.
The pink salt $(NH_4)_2SnCl_6$ is tin-based compound that occurs naturally in volcano ashes. When its ethanol solution gets in contact with tin alloys, it accelerates the tin pest process. The mechanism of the acceleration has not been explained, yet. One suggested sequence is i) precipitation of grey (alpha) tin from the solution on the alloy surface, ii) the precipitates function as inoculator and iii) progress of phase transformation.

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Possible Tin Pest Blocking by Addition of Au in Sn Alloy

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Low content alloys (impurities in Sn) have a significant effect on the course of tin pest. However, their influence, like the degradation of tin, is described insufficiently and sometimes even with seemingly contradictory results. The proven slowing of the tin plague process is achieved by alloying by a small amount of Pb (0.01 %) or according to the literature by the addition of Bi, Ag and Au. However, it is abandoned from Pb due to toxicity and Bi is a very rare element on the ground that is not resistant to the action of hydrochloric acid. Ag promotes the formation of so called Sn whiskers that reduce the electrical properties of the material. Au is already used in conjunction with Sn for smaller electrical parts, and if it turns out that the limit amount is already sufficient to block the pest, the financial demands in the production of larger equipment (for example solar cells) would be acceptable. Therefore, model alloys with the limit concentration of Au in Sn were prepared and the course of the tin pest was observed under defined conditions. This research is supported by the IGA UCT grant (A2_FCHT_2024_080).

High-strength 18Ni300 Maraging Steel Prepared by Spark Plasma Sintering

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The present work demonstrates a novel approach for the compaction strategy for the 18Ni300 high-strength maraging steel using a Spark Plasma Sintering (SPS) technique. Furthermore, the influence of two heat treatment modes on the structure and properties of the as-produced materials is examined. It was found that the higher temperature of the SPS process has caused the formation of less defective and more ductile material. Optical and scanning electron microscopy were used to examine the microstructure of the as-produced and heat-treated samples. The phase composition was determined using X-ray diffraction analysis. Microhardness measurements and tensile tests at laboratory temperature have shown that heat treatment causes the strengthening of the studied material. The type of the strengthening phases was investigated using transmission electron microscopy. Additionally, the obtained results are compared to the results of conventionally prepared 18Ni300 maraging steel.

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Heat treatment of additively manufactured high-strength maraging steel

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Maraging steels are high-alloyed steels with very low carbon content featuring a great combination of mechanical properties and ductility. Their superior strength is caused mainly by precipitation hardening, usually after standard aging treatment at around 480 °C. Specifically, 1.2709 maraging steel (i.e., 18Ni-300) is one of the metallic materials frequently used for additive manufacturing, especially by the most widely used selective laser melting. 3D-printed metals typically showcase different, very fine microstructures compared to conventionally manufactured ones. For this reason, the influence of various aging conditions was mapped on the additively manufactured material, both on samples in as-printed and post-print solution-annealed (after 820 °C/1 h) states. The subsequent aging treatment was held under three temperatures (440 °C, 490 °C and 540 °C) and a total of five durations (2, 4, 6, 8 and 10 h). The material before and after aging was studied from the microstructural point of view, as well as phase composition and finally microhardness. A common phenomenon of austenite formation in the martensite matrix–having a detrimental effect on the mechanical properties–was found to be related to both the manufacturing and the heat treatment processes.

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Structure-Property Correlation in Lithium Borophosphate Glasses Modified with Niobium Oxide

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Borophosphate glasses of the series $(100-x)[0.4Li_2O-0.2Nb_2O_5-0.4P_2O_5]-xB_2O_3$ were studied in a composition range of x = 0-48 mol% B_2O_3. Basic physical properties were determined, and thermal properties studied by differential thermal analysis, thermomechanical analysis. The glass structure was investigated using Raman spectroscopy and ^{11}B and ^{31}P MAS NMR. The electrical properties of the glasses were obtained by using impedance spectroscopy.

Focus of this contribution will be given on MAS NMR analysis of studied glasses. Structure of the glasses was probed with multiple MAS NMR experiments. To get first information about the glass structure, standard 1D experiments of ^{11}B and ^{31}P nuclei were performed. To probe interconnections between phosphate and borate species was further studied by 2D correlation techniques. Namely $^{11}B\{^{31}P\}$D-HMQC sequence to investigate P–O–B connections. By combining all these methods, we were able to prepare an approximate structural model of these glasses, which could be used to explain the macroscopic properties of the studied glasses.

Influence of Solution Composition and *In Vitro* Test Arrangement on the Results of Potential Bioactivity of Bioactive Glass 45S5

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The bioactivity of glass materials tested *in vitro* is not only influenced by the reactivity of the material itself but also by the composition of the test solution. Usually, these tests are carried out in a simulated body fluid (SBF) and provide valuable insight into how the material interacts with physiological fluids in a living system.

This study aimed to observe the bioactive behaviour of glass particles based on Bioglass 45S5 in three different testing solutions: a) TRIS-buffered SBF (ISO 23317:2014) as a reference, b) non-buffered SBF, and c) non-buffered SBF with a concentration of $(HCO_3)^-$ 15 $mmol \cdot dm^{-3}$. The experiment was conducted under static-dynamic conditions for the duration of four days. Biomineralization process was monitored throughout the experiment. Eluate analyses, including pH levels and element (Si, Ca, P) concentrations measured by ICP-OES, as well as material analyses (weight changes, SEM/EDS, XRD), were performed.

The findings show that samples immersed in TRIS-buffered SBF exhibit notably accelerated dissolution rates compared to those in unbuffered SBF solutions. Samples exposed to SBF with modified $(HCO_3)^-$ ion concentrations displayed similar trends, albeit with marginally decreased levels of Ca, P, and Si concentrations relative to samples in unbuffered SBF.

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Biodegradable zinc-based materials prepared by powder metallurgy processes

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Introduction

Zinc has garnered attention as a promising biomaterial, credited to its exceptional biocompatibility and resistance to corrosion. Despite these advantages, its mechanical properties and bioactivity remain areas of concern, limiting its applications. Recent research efforts have concentrated on enhancing zinc's properties by introducing additional elements (such as copper and manganese), altering its microstructure, and employing diverse surface treatments during preparation. These methodologies have encouraging outcomes in improving mechanical properties and bioactivity at elevated temperatures. The trajectory of zinc-based biomaterials points towards the innovation of novel alloy compositions and preparation techniques tailored to enhance their suitability for specific biomedical applications.

Methodology

Our research is oriented on fabricating of nano-grained zinc materials utilizing powder metallurgy methodologies, particularly mechanical alloying (MA), followed by rapid compaction techniques such as spark plasma sintering (SPS) in conjunction with extrusion. Prepared materials were observed by optical and scanning electron microscope, chemical composition was determined by X-ray analysis and mechanical properties were tested by tensile testing.

Results

Through the selection of processing parameters and incorporation of alloying elements, we attain a compact microstructure characterized by uniformly dispersed intermetallic phases. Grain refinement, combined with solid solution strengthening, serves to improve mechanical properties. Nonetheless, remnants of oxide particles originating persist within the microstructure, potentially heightening the susceptibility to brittle fractures.

Conclusion

Based on our research, materials subjected to extrusion and exhibiting texture demonstrate enhancements in mechanical properties. However, further studies are necessary for possible applications of these materials.

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Antimikrobiální úpravy textilních materiálů – přání a skutečnost

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Úvod

Přednáška se zabývá antimikrobiálními úpravami textilií, kde v úvodu budou probrány možnosti těchto úprav, jak jsou nabízeny v odborné literatuře a na trhu. Textiliemi se zde rozumí nejen materiály pro denní nošení a materiály pro personál nemocnic, vojenských a bezpečnostních složek, ale i obvazy, bandáže a kryty ran.

Ve druhé části přednášky budou představeny materiály vyvinuté na Fakultě chemicko-technologické, Univerzity Pardubice, způsob jejich přípravy a naměřené výsledky jejich antimikrobiální účinnosti. Tyto výsledky budou porovnány s materiály nabízenými na trhu.

Metodika

Antimikrobiální účinnost materiálů byla testována difuzní agarovou metodou, která slouží ke kvalitativnímu posouzení antimikrobiálního účinku u testovaného materiálu. Zjišťuje průměr inhibičních zón kolem daného vzorku a tím zároveň zjišťuje citlivost určitého mikroorganismu k danému vzorku materiálu. Dále se dá touto metodou také určit, zda má určitý mikroorganismus baktericidní či bakteriostatický účinek.

Testované mikroorganismy: *E. coli, Pseudomonas aeruginosa, Enterococcus faecalis, St. aureus, Candida albicans.*

Výsledky a závěry

Ve třetí části přednášky budou zhodnoceny postupy, které vedou ke skutečně antimikrobiálně účinným materiálům, a technologické možnosti jejich výroby.

Grantová podpora

Práce byla zčásti finančně podpořena projektem TP01010012 - Rozvoj systému podpory projektů proof-of-concept na Univerzitě Pardubice, GAMA2-01/002, Technologická agentura České republiky.

Degradation of a new clinker-free calcium sulfate binder 3C due to freezing and thawing

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Due to today's global need to reduce CO_2 emissions, new hydraulic binders with the potential to replace Portland cement in the future are being prepared. Clays calcined in the range of 500-900 °C are a promising low-emission source of pozzolans, which can significantly contribute to further reducing the impact on the environment. The combination of calcined clays with calcium sulfate and lime creates a new stable calcium sulfate hydraulic binder called 3C with suitable cement-like mechanical properties. However, for a new binder, it is necessary to observe its behaviour in corrosion conditions, which are one of the most important properties for the construction industry.

The aim of this project was to describe the behavior of the 3C binder under conditions of alternating freezing and thawing (FT) in the presence of water or chemical deicing agents according to the ČSN EN 73 1326 standard. First, a set of slurries and mortars of the 3C binder with different ratios of components was prepared. A constant water to binder ratio as well as plasticizer addition were used. Cylindrical samples with a minimum height of 50 mm were prepared using polypropylene pipes with a diameter of 100 mm. After a month of curing, water or a 3% NaCl solution was poured onto the sample surface. Subsequently, the samples were cycled at alternating temperatures according to ČSN EN 73 1326. After every 25 FT cycles, the amount of surface waste was weighed. The selected samples were analyzed from the point of view of phase changes by the XRD method. The results were compared with reference cement samples prepared with the same water to binder ratio.

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Hydrophobic Heteroboroxine-Based Materials

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Nowaday, a great attention is focused on the development of hydrophobic coatings. In addition to the traditional materials such as silanes, silicones and fluorinated polymers, inorganic-organic hybrid materials that combine the of the inorganic and organic component are currently being studied. Recently, a transparent superhydrophobic coating was fabricated using N-Boroxine-PDMS and SiO_2 nanoparticles showing water contact angle WCA = 160°.[1]

Considering that our group is engaged in the study of N→M intramolecularly coordinated heteroboroxines (HBOs)[2] having the central six membered ring MB_2O_3 (M = Ge and Sn), the goal of this research is to study their hydrophobic properties.

First, we tested the formulations composed of linear, or star-shaped, PLAs, PCLs and PVLs and stanna-boroxines $L(Ph)Sn(O_3B_2(4\text{-}CF_3\text{-}C_6H_4)_2$ and $L(Ph)Sn(O_3B_2(3,5\text{-}(CF_3)_2\text{-}C_6H_4)_2$ ($L = \{2,6\text{-}(Me_2NCH_2)\text{-}C_6H_3\}^-$) as additives. Further, the Lewis acidity of boron atom in these fluorinated stanna-boroxines allows to form N→B coordination bond with N-bases. Based on this, we syntesized coordination polymers derived from poly(4-vinylpyridine) and poly-(4-vinylpyridine-*co*-styrene). Finally, HBOs have also been incorporated into oligomeric or polymeric chains by Shiff-coupling of $L(Ph)Sn(O_3B_2(4\text{-}CH{=}O\text{-}C_6H_4)_2$ and $LGe(O_3B_2(4\text{-}CH{=}O\text{-}C_6H_4)_2$ with various diamines such as 1,4-benzenediamine, ethylenediamine or amine-terminated siloxane.

For the determination of the hydrophocity, thin layers of prepared formulations and materials were fabricated by spin-coating method on silicon wafer, glass and PE and WCAs were measured by sessile drop method. The surfaces were further characterized using SEM and AFM to check the morphologies of the layers.

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Preparation and characterization of thin films for new generation of cutting tools

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Introduction

Nitride thin films based on aluminium and titanium, prepared by arc evaporation, are widely employed to enhance the durability and performance of machining tools. Their exceptional mechanical properties are strongly dependent on phase composition and deposition parameters. In this context, the cubic phase exhibits superior properties when compared to the hexagonal phase. Stabilization of the cubic phase by adding new elements and altering deposition parameters was studied in this work. Thin films were investigated to determine their elemental and phase composition along with their mechanical properties.

Methodology

Aluminium-titanium nitride thin coatings were deposited by cathodic arc evaporation in HTC650 equipment from Hauzer Techno Coating. The targets used in this experiment were prepared by powder metallurgy with an atomic ratio of aluminium to titanium set at 67/33 at. %. Phase composition was identified by X-ray diffraction. Microstructure was studied on an optical microscope (Nikon Eclipse MA 200). More detailed observation was done using a scanning electron microscope (Tescan Lyra 3), equipped with energy dispersion spectroscope (Oxford Instruments, 80 mm2). Adhesion was tested by Daimler-Benz test using a HPO250 Rockwell hardness tester, while the microhardness was measured using Future-Tech FM-700. The tribological properties were determined by the Tribotechnic TRIBOtester machine.

Results

High hardness above 35 GPa has been achieved by (Al0,67Ti0,33)N coatings with the majority of cubic phase, prepared by arc evaporation with different deposition parameters.

Conclusion

This research documents the influence of deposition parameters on phase formation and mechanical properties of widely used (Al0,67Ti0,33)N thin films prepared by cathodic arc evaporation.

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Ge-Sb-Te thin films fabricated by co-sputtering and pulsed laser deposition

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During the last decades, the thin films from GeSbTe (hereinafter GST) or AgInSbTe system have been deeply investigated. The main reason for high scientific interest in this class of materials is the fact that these materials are able to transform quickly and reversibly from amorphous to crystalline phase (disorder-order transition) and vice versa; this phenomenon was first reported by Ovshinsky [1]. Phase transition can be reversibly switched by varying the electric field or temperature when heating is done using a laser pulse in optical recording applications. The unique characteristics of phase change GST materials are based on huge optical reflectivity (up to 30%) or electrical conductivity (several orders of magnitude) changes proceeding upon phase transition.

The aim of this work is to combine co-sputtering and pulsed laser depozition as an advanced techniques for thin films growth with the fabrication of an important class of inorganic materials being represented by GST thin films. The characterization of deposited thin films in as-deposited state (amorphous phase) as well as in crystalline state (induced by thermal annealing) was performed exploiting atomic force microscopy, scanning electron microscopy with energy-dispersive X-ray analysis, X-ray diffraction, electrical resistivity, and variable angle spectroscopic ellipsometry data. The results are discussed in relation with the chemical composition of the fabricated GST thin films.

[1] S. R. Ovshinsky, Phys. Rev. Lett., 21, 1450-1453 (1968).

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Properties of a novel lignin-based urea formaldehyde resin as an adhesive for wood and wood composites

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Lignin, produced in pulp mills around the world, is primarily used as a source of energy. Due to its chemical properties, there is potential for developing lignin-based materials. The current focus is on the development of adhesives from lignin, with an emphasis on lignosulfonate due to its superior reactivity compared to kraft lignin. However, kraft lignin is much more widely produced worldwide.

In this study, kraft lignin was used as a partial replacement for preparing urea-formaldehyde resin for bonding wood and wood-based composite materials. UF resins with 0 to 50% lignin replacement were prepared. The tensile shear strength of glued joint on high density fibreboard (HDF) samples was tested for the developed resins. The shear strength results show that the shear strength decreases with increasing lignin content. At the same time, a significant decrease occurred with the addition of 50% lignin due to too high viscosity of the prepared resin. After the test, the failure condition of the glued joint was visually evaluated.

Metallic and polymer-composite bipolar plates for PEMFC

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Introduction

Proton exchange membrane fuel cells (PEMFCs) are a promising alternative to combustion engines in automotive next to Li-on batteries. PEMFCs have future also in heavy duty transportation, trains and aircrafts where there are higher demands and longer development time. PEMFC consist of several main parts such as Membrane Electrode Assembly (MEA), catalyst, Gas Diffusion Layer (GDL) and Bipolar Plates (BP). In addition, BPs have distribution channels manufactured inside. The most important roles of BPs are distribution of gases inside PEMFC, heat dissipation, current collection and water management. Therefore, there are many requirements for mechanical, corrosion and conductivity properties.

Methodology

The U.S. Department of Energy (DOE) lists requirements for bipolar boards. The target corrosion and conductive properties also have their standardized tests. For corrosion testing, a simulated PEMFC environment and corresponding potentiostatic (PS) or potentiodynamic (PD) polarization at elevated temperature is used. Conductivity in the form of interfacial contact resistance (ICR) is measured in the initial state and after 24 hours of PS. The ICR is measured at an applied force of 138 $N \cdot cm^{-2}$, which corresponds to realistic conditions.

Results

Most used metallic material for BPs in PEMFC is either titanium or stainless steel (AISI 316L). Both have excellent corrosion properties in simulated PEMFC environment due to the passive layer on the surface. The passivation is the reason for very poor surface conductivity in both cases. Therefore, titanium surface was succesfully enhanced to improve conductivity and the ICR decreased by the factor of four. AISI 316L was coated using polymer-composites resulting in great corrosion properties and also improvement in the terms of ICR.

Conclusion

Metallic BPs are better than graphite in transport, mainly due to their better mechanical properties. The issue is the stability in the environment, meaning maintaining good conductivity and low corrosion during the lifetime of the PEMFC. Surface treatments and coatings help improve the performance of Titanium and AISI 316L.

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ADVANCEMENTS IN LIGHTWEIGHT MAGNESIUM ALLOYS WITH HIGH RESISTANCE TO IGNITION

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Introduction

While magnesium alloys are among the lightest metal structural materials, their previous restriction in aircraft cabins stemmed from safety concerns, primarily due to magnesium's high reactivity, which makes it susceptible to corrosion and flammability. However, recent advancements have enabled the modification of these alloys to meet safety standards by significantly enhancing their mechanical, corrosion and oxidation properties through alloying.

Methodology

Magnesium alloys with the elemental composition Mg-Y-Al-Ca were prepared, followed by an investigation into the relationship between material structure and ignition resistance. Microstructural analysis was conducted using SEM, EDS, and XRD techniques. The ignition temperature was determined via thermal analysis, and subsequent studies focused on oxidation properties.

Results

Novel magnesium alloys were developed exhibiting enhanced resistance to ignition compared to commercial materials. These alloys successfully passed flammability tests under laboratory conditions, demonstrating increased ignition resistance and suppressed flammability.

Conclusion

A promising alloy has been developed that withstands flammability testing in laboratory settings. Further investigation or testing could include it among the candidates for suitable alloys for use in aircraft cabins.

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BIOMASS ASH AND ITS UTILIZATION POSSIBILITIES FROM THE PERSPECTIVE OF CIVIL ENGINEERING

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The energy sector has been preparing for a transition from coal combustion to purely green energy sources in recent years. This brings changes that have, and especially in the future will have, a significant impact on the construction industry. The combustion of coal produces non-combustible residues – fly ash, which is widely used in construction and is an integral part of, for example, blended cements and concretes. Currently, there is a large-scale shift towards the combustion or co-combustion of biomass with coal. The resulting non-combustible residue – biomass ash (BMA), exhibits different chemical and phase compositions, making its utilization in construction significantly more complex.

This work aims to present the possibilities of using products from the combustion of biomass in large sources and simultaneously highlight the wide differences in the chemical and phase composition of these products. The paper clearly outlines the requirements for ashes for construction purposes and evaluates critical parameters from the perspective of biomass ashes.

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POROUS TI-6AL-4V PARTS PRODUCED BY SELECTIVE LASER MELTING

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Titanium alloys, especially Ti-6Al-4V, are the most widely used materials for medical applications such as dental or orthopedic implants. When applied as an implant, a negative stress-shielding effect can develop. The stress shielding effect originates from a different elastic modulus between the bone and the implant. The negative effect can be reduced by using porous implants which also improve and accelerate the binding of the implant with bones. A porous structure with minimal need for post-production machining of the surface can be produced by selective laser melting (SLM). The SLM technology is the most preferred approach for metal 3D printing because of its many advantages compared to conventional methods. In this study, as-built and as-built plus heat-treated samples made from Ti-6Al-4V alloy printed by SLM are tested. Microstructure was observed using light optical and scanning microscopy (LOM and SEM, respectively). Porosity was calculated using ImageJ software on LOM micrographs of cross-sections of the samples. Furthermore, mechanical properties such as ultimate compressive strength and microhardness HV0.1 were measured.

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CHARACTERIZATION OF HYDROXYAPATITE POWDERS FOR 3D PRINTING APPLICATIONS

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Additive manufacturing continues to evolve with the introduction of novel materials and advancements in specialized applications. One such area of focus is 3D printing in dentistry, where hydroxyapatite (HAP), a ceramic material, is gaining traction for filament production.

This study explores the initial step in filament manufacturing: the analysis of specific powder properties. Three distinct HAP powders were evaluated for particle size distribution, compressibility, and flow properties. Understanding these properties is crucial for predicting the material's behavior within the extruder and ultimately achieving a homogeneous filament suitable for further processing.

Furthermore, the analysis of mechanical properties is highlighted as another key parameter for potential application in Finite Element Method (FEM) simulations. This comprehensive approach provides valuable insights for optimizing the 3D printing process of hydroxyapatite filaments for dental applications.

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The impact of nitrogen implantation on the biodegradable Zn-0.8Mg-0.2Sr alloy

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Biodegradable materials have garnered significant attention worldwide due to their potential advantages in enhancing patient comfort. Recent research has focused on surface modifications aimed at improving the interaction between implants and tissues. In this study, the surface of the biodegradable Zn-0.8Mg-0.2Sr alloy was implanted with nitrogen ions, and the impact of this process on the microstructure was observed. Additionally, pure phases occurring in the alloy microstructure were also subjected to implantation. The findings revealed the formation of nanopore structures on the surface of pure zinc and the development of cracks in the Mg_2Zn_{11} intermetallic phase. In the case of the alloy, a combination of these effects was observed, along with the identification of regions with varying heights through AFM measurements. The sputtering yield was calculated using the TRIM code, and the results were found to be in good agreement with previous findings, highlighting direct influence of sputtering on surface roughness. Furthermore, slight changes in the chemical composition of the surface were observed, particularly in the formation of oxides. Specifically, the presence of Mg_3N_2 was confirmed through various measurements such as XRD and TEM. However, the stability of nitrides over time was found to be limited, lasting only several hours post-implantation due to their susceptibility to humid environments. Based on these results, potential benefits could be identified for the preparation of active surfaces on the Zn-based material.

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CORROSION PROPERTIES AND BOND STRENGTH IN CONCRETE CONVENTIONAL PRESTRESSING STEEL REINFORCEMENT WITH PLASMA SPRAYED SiC COATING

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Corrosion damage to conventional prestressing reinforcement placed in a grout channel stimulated with chloride anions can lead to unpredictable collapse of reinforced concrete structures. An expert report previously carried out on the condition of the Troja footbridge after its collapse indicated that corrosion of the prestressing reinforcement stimulated by chloride anions was the cause. In this paper, the possibility of applying corrosion protection in the form of a protective SiC-based plasma coating is studied. The barrier protection properties of the silicon carbide coating partially incongruently decomposed into elemental silicon and amorphous SiO_2 were comparatively verified in hydrochloric acid - AAS solution by analyzing the iron content of the test solution after the exposure time. Furthermore, the bond strength of the reinforcement coated in this way with concrete of normal strength was verified by means of a pull-out test. Testing was carried out on standard cubic specimens with standard uncoated and ceramic coated reinforcement applied. Interpretation of the bond strength test results included measurement of changes in surface roughness (R_a) and contact surface angle of the coated ceramic.

REACTIONS OF SILICON CARBIDE IN WATER-STABILIZED PLASMA

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SiC silicon carbide has a set of extreme physicochemical properties that predispose it to applications in almost all industries. At normal or slightly elevated temperatures it is used in engineering as a grinding or machining material, it is used in optics, electronics, electrical engineering, etc. Its high corrosion resistance and especially its radiation stability are also used in the construction of equipment in contact with nuclear fuel or directly in nuclear reactors. However, the behaviour at extremely high temperatures is problematic, with oxidation, phase or structural transformations and incongruent thermal decomposition (which may have been one of the causes of the Fukushima nuclear accident). However, published data on these quantities are highly inconsistent, as the study of materials at temperatures above 3000 K is experimentally difficult. In this paper, the behaviour of SiC in a plasma generated in a hybrid water-stabilised WSP®-H 500 plasma torch is described, which can reach temperatures up to 25 000 K at its output. The products formed in air or nitrogen protective atmosphere during plasma deposition of powdered SiC on graphite substrates are described and studied. As a partial result, it is possible to clarify the differences between passive and active oxidation of SiC, justified in the literature by the existence of volatile and unstable SiO molecules.

SEPARATION OF SCANDIUM AND THORIUM FROM RARE EARTH MINERALS

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Both uranium ores and the thorium-bearing phosphate mineral monazite contain significant amounts of lanthanides, including scandium and yttrium. Similar variations have been identified following the recent announcement of the discovery of new lanthanoid deposits in the Kiruna region of Sweden. The processing of raw materials to extract REEs and scandium primarily requires the removal/isolation of radioactive thorium. This can be achieved by, inter alia, carbidation of the raw material, with subsequent conversion of the hydrolyzable carbides into soluble compounds suitable for ion-exchange separation. The possibility of formation of thorium carbide by reaction with carbon at temperatures of 2000 - 2200°C by Spark plasma sintering (SPS) was verified on raw material from the Czech uranium deposit Jáchymov, containing oxides and silicates of scandium and thorium, with high radioactivity caused by thorium content. At a maximum temperature of 2200°C in the FCT SYSTEME HP-D10 apparatus, hydrolyzable carbides Sc_2OC and Sc_4C_3 were formed, and carbidation of the present ThO_2 did not occur, even when using the more reactive carbon form of graphene. A thermodynamic calculation of the reaction $ThO_2 + xC = ThC, ThC_2 + yCO$ indicated the possibility of this reaction above 2500°C. The reaction at higher temperatures was therefore verified in an Acheson-type micropiece with a tungsten heating core with the possibility of reaching temperatures up to 3400°C. After hydrolysis of this product, allylene, a typical hydrolysis product of scandium carbides, was identified in the gas phase. After subsequent dissolution of the sample in hydrochloric acid and filtering of the solution, only the radioactive monocarbide ThC (type B1) was identified in the insoluble residue. The radioactivity value of the leachate after removal of the thorium, suitable for further safe processing, was at the limit of the exemption level according to the SÚJB standard.

Properties of austenitic stainless steel containing yttrium oxide

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Introduction

Improving the mechanical characteristics of traditional materials is possible by incorporating ultrafine oxide particles, which suppress dislocation movement, consequently bolstering material strength. This approach is applicable to austenitic steels, resulting in enhanced strength and resistance to creep, and suitability for high-temperature uses. Understanding the formation and arrangement of dispersed oxides in metal alloys is essential for the development of innovative high-strength materials.

Methods

The process of preparation of oxide dispersion-strengthened austenitic steel 316L included mechanical alloying of austenitic steel powder with Y_2O_3. During the mechanical alloying phase, elemental Y was introduced to dissolve within the Fe matrix as an alternative approach. Subsequently, these powder precursors were compacted through Spark Plasma Sintering (SPS), followed by a detailed analysis of their microstructure. The resulting compacts were then subjected to an assessment of their mechanical properties.

Results

Initial observations indicate a tendency for the formation of chromium-containing carbides, believed to result from the minor diffusion of carbon originating from graphite tools utilized in the procedure. Moreover, it was noted that both Y_2O_3 and Y could be successfully incorporated into a solid solution during the mechanical alloying stage, with subsequent precipitation during compaction. The mechanical characteristics of the materials exhibited variability, influenced not only by their chemical composition but also by the precise conditions employed in the Spark Plasma Sintering (SPS) process.

Conclusion

Materials with homogeneously distributed Y_2O_3 particles have been successfully prepared by powder metallurgy. Further research will focus on optimizing the SPS conditions to avoid carbide formation in prepared materials.

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Corrosion Effect of Organic Buffers on Bioactive Glass

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The Simulated Body Fluid (SBF) is used for *in vitro* testing and its preparation is described in the ISO standard 23317:2014. Previous studies have showed that the TRIS buffer, which maintains the pH in SBF, accelerates the dissolution of bioactive glass/glass-ceramics and helps precipitate a hydroxyapatite (HAp) layer.

This work aimed to study the corrosion behavior of the TRIS and HEPES buffers and compare the rates of the bioactive glass dissolution, as well as their effect on the HAp formation.

Bioactive glass samples, in the form of bulk, were tested under the static-dynamic conditions by the solutions: i) SBF without TRIS buffer (**SBF**), ii) **SBF+TRIS** (ISO standard) and iii) **SBF+HEPES**. The concentrations of the elements (Ca, P and Si) in eluates were analysed using ICP-OES. The pH was measured by glassy electrode at the physiological temperature (36.5°C). Glasses and newly formed layers were observed by SEM/EDS and XRD methods.

This work confirmed that TRIS and HEPES buffers used in SBF produced false positive results of *in vitro* tests. Moreover, the chemical composition, morphology and crystallinity of newly created apatite layer formatted in buffered SBF are different

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Preparation of transition metal carbides with usage of carbon waste precursours

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Introduction

Carbides of transition metals have a unique combination of properties such as high melting points, high values of Young´s modulus of elasticity, extreme hardness and good chemical stability. Due to this combination, these materials have broad usage like machining tools and protective coatings for extreme environments like the nuclear industry. Carbides can be prepared by mechanical alloying using the carbon waste made during pyrolysis of polypropylene, yielding also carbon 2D forms. This method provides the preparation of ultra-fine grains of carbides due to mechanical alloying with decreasing technological and economical demandingness. The goal of this work was the preparation of tungsten and titanium carbides by mechanical alloying. For the preparation, the milling time was determined based on the kinetics of carbide formation. The effect of carbon excess on the kinetics of formation was studied as well as the mechanical properties of sintered carbide powders. Further, the powder carbides will be used in high entropy alloys and determination of their effect in these alloys.

Methodology

Preparation of powder carbides by mechanical alloying method. Description of powder carbide formation in respect of mechanical alloying by XRD, XRF, SEM + EDS method.

Results

In this work, the effect of n-heptane used as a process control agent on the preparation of WC or TiC powder carbides was studied. It was confirmed that n-heptane significantly affects the carbide formation. The excess of carbon, as well as the content of n-heptane, is prolonging the formation of carbides.

Conclusion

In this work, the WC and TiC powder carbides were prepared. Also, kinetics of carbide formation were studied based on mechanical alloying time. The effect of n-heptane used as a process control agent and excess of carbon was studied. Both of these chemicals are decreasing the speed of carbide formation.

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Microstructure of super duplex stainless steel prepared by powder metallurgy and additive technology

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Duplex stainless steel (DSS) offers a unique combination of properties, including excellent corrosion resistance, high strength, good toughness, ductility, and fatigue resistance. The microstructure of this steel should consist of a balanced ferrite-austenite ratio. The phase composition depends on the chemical composition of the material and the applied heat treatment. DSS is usually heat-treated by solution annealing to achieve the required ferrite-austenite microstructure without secondary phases. In this study, the microstructure and mechanical properties of super duplex stainless steel SAF2507, consolidated via Spark Plasma Sintering (SPS) and deposited by Directed Energy Deposition, were investigated. Both techniques are able to produce samples with nearly equal ferrite-austenite microstructure in the as-built state. The yield strength of SPS-ed steel reached the value of 550-600 MPa, while the yield strength of DED-ed ranged from 600 MPa to 680 MPa.

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CHARAKTERIZACE POVLAKOVANÉ BIODEGRADABILNÍ SLITINY Zn-0,8Mg-0,2Sr

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Výzkum biodegradabilních kovových materiálů se v současnosti zaměřuje na zlepšení povrchu implantátů, který by podpořil rychlejší hojení kostí. Biodegradabilní materiály se v lidském těle postupně rozkládají, a proto by potenciální implantát neměl obsahovat toxické kovy. Z tohoto důvodu se nejčastěji pro přípravu biodegradabilních materiálů používají Mg, Zn a Fe. Problémem těchto prvků je ale jejich rychlost degradace a biokompatibilita, což by mohlo být vyřešeno povrchovou úpravou implantátu. V této práci je komplexně popsán mechanismus vzniku hopeitu na biodegradabilní slitině Zn-0,8Mg-0,2Sr, která se řadí mezi perspektivní materiály pro biomedicínské účely. Výzkum je zaměřen na chemické složení povlakovací lázně, dobu expozice a teplotu, které ovlivňují strukturu, kvalitu, distribuci, fázové složení, tloušťku a drsnost vzniklé vrstvy. Byly nalezeny podmínky povlakování, při kterých vznikla hladká a rovnoměrně distribuovaná vrstva hopeitu. Dále byl ukázán vliv přítomnosti hopeitu na interakci slitiny s buňkami a bakteriemi. Přítomnost vrstvy hopeitu se projevila zvýšenou viabilitou buněk během přímého testování cytotoxicity. Vznik hladší vrstvy pozitivně ovlivnil antibakteriální vlastnosti. Výsledky jsou tedy nadějné pro použití povlakované biodegradabilní slitiny Zn-0,8Mg-0,2Sr jako dočasného implantátu.

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VLASTNOSTI LAMINÁTŮ S ANORGANICKOU MATRICÍ V ZÁVISLOSTI NA TEPLOTĚ VYTVRZOVÁNÍ

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Byly připraveny lamináty s uhlíkovými vlákny a anorganickou matricí, které se lišily teplotou vytvrzování (5 °C, 10 °C, laboratorní teplota a 65 °C). Jako anorganická matrice bylo použito geopolymerní pojivo připravené z hlinitokřemičitanu (kalcinovaný kaolinitický jílovec) a alkalického aktivátorů (roztok draselného vodního skla s hydroxidem draselným). Použitá uhlíková vlákna byla amorfního charakteru. U připravených laminátů byla testována pevnost v tahu po vytvrzení za laboratorní teploty a po vystavení vysokým teplotám (400 °C a 600 °C). Byly porovnány naměřené hodnoty pevnosti v tahu všech laminátů, z kterých vyplývá, že nejlepších pevností v tahu dosahují lamináty s anorganickou matricí se sníženou rychlostí tuhnutí při 5 °C.

Selective laser melting of binary Ti-30Nb alloy from an elemental powder mixture

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Introduction

Selective Laser Melting (SLM) is one of the additive methods for the manufacturing of metallic materials and belongs to powder bed fusion technology. The final product is sintered by a laser beam, layer by layer, based on a computer model. Beta titanium alloys are considered as an adequate substitution for the currently most used Ti-6Al-4V alloy for the production of implants, as they contain only non-toxic alloying elements and have a lower modulus of elasticity. The modulus of elasticity of the beta alloy is closer to the modulus of elasticity of cortical bone, thus reducing the risk of the so-called stress shielding effect. In this work, a binary beta titanium alloy Ti-30Nb prepared directly from a mixture of elemental powders was studied. The effect of process parameters on the porosity and structure of the material was evaluated and the mechanical properties of the printed alloy were determined.

Methodology

Laser diffraction, optical and scanning electron microscopy, XRD, compression tests, Vickers‘ hardness

Results

A binary Ti-30Nb alloy was successfully prepared by SLM from a mixture of elemental powders. According to the printing parameters, the porosity of individual samples and the content of undissolved niobium particles varied. In terms of mechanical properties, the samples achieved very good compressive yield strength and hardness.

Conclusion

The obtained results showed that different melting temperatures of the individual powders do not allow the preparation of a homogeneous material. The Nb particles remain undissolved in the structure and their content is higher, the lower the laser energy density is applied. However, when a higher laser energy density is used, partial evaporation of the material and the formation of larger spherical pores due to excessive melting occurs. Despite the inhomogeneities in the structure, the alloy reached very good compressive yield strength and hardness.

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Applied catalysis and organic technology

Highly Active Pt/*Y*-carbon Catalyst in Hydrogenation of Benzene

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Wet impregnation of Pt salt solution on zeolite-templated carbon (ZTC) used faujasite zeolite as a hard template provided Pt/*Y*-carbon catalysts. This can be prepared with a very wide range of metal loadings up to at least 25 wt.% with very good dispersion of the metal particles comparable to the loading for materials with 3 wt.% Pt. Due to the 3D-organised open porous structure that allows access to the active centres, the TOF_{Pt} values are identical even for very large Pt loadings. The catalytic activity of the Pt/*Y*-carbon is thus directly proportional to the Pt loading, and the high concentration of active Pt sites results in extraordinarily high activities in the hydrogenation of benzene to cyclohexane. The Pt nanoparticles supported on zeolite-templated carbon are an example of a new class of ZTC metal-supported catalysts that provide a very large concentration of metal sites on a readily accessible 3D-organized porous support. A detailed description of the research results is given by Rastegar et al.[1]

Acknowledgments
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Extraktivní recyklace textilií

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Ve své práci jsme se zabývali problematikou recyklace textilií, konkrétně extraktivní separací složek z textilních směsí bavlna/polyester. Bylo experimentálně prozkoumáno několik možných metod separace. První metodou bylo rozpouštění bavlněných vláken a jejich zpětné vysrážení v podobě regenerovaných celulózových vláken, druhou metodou byla hydrolýza polyesterových vláken ve vodném roztoku hydroxidu sodného, třetí metodou byla methanolýza polyesterových vláken v přítomnosti vhodných katalyzátoru a rozpouštědla dichlormethanu a čtvrtou a poslední metodou byla methanolýza polyesterových vláken v přítomnosti katalyzátoru kyseliny paratoluensulfonové.

Jako vhodná metoda separace pro průmyslové využití se jeví methanolýza v dichlormethanu s katalyzátorem uhličitanem draselným, která umožnila separaci veškerých polyesterových vláken z textilní směsi.

Electron Tomography as a Powerful Tool for Detailed Investigation of Catalysts Microstructure

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This work deals with the preparation and use of electron tomography methodology at UCT Prague. The work is divided into a part dealing with the methodology of electron tomography and a part dealing with case studies of catalysts tomography. The methodology of electron tomography consists of the preparation of a specimen suitable for electron tomography (for example: FIB-SEM lift-out method), the acquisition and processing of tomographic data taken in a transmission electron microscope, and the quantitative evaluation of the acquired image data of the catalyst. The case studies are used to demonstrate the capabilities of electron tomography as a tool for material study. In addition to the 3D model, the reconstruction also results in quantitative information about the material, such as particle size distribution, distance of metallic parts from the material surface, or the connectivity of porous systems. Based on the information obtained, it is possible to observe a change in pore connectivity, sintering, or migration of metal on the porous support.

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Heterogeneous catalysts based on quaternary nitrogen salts

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Salts derived from nitrogen-based compounds have a broad range of applications in chemistry, from organic synthesis to electrochemistry. One particularly promising application is their use as organocatalysts for various chemical transformations, such as the cycloaddition of carbon dioxide to epoxides and the Knoevenagel condensation. The cycloaddition of carbon dioxide to epoxides represents a significant synthetic route for the production of cyclic carbonates, which are utilized as precursors for polymer and fine chemical preparation. Carbon dioxide serves as a non-toxic, cheap, and renewable carbon source. While, the Knoevenagel condensation reaction is a versatile method for the synthesis of *α,β*-unsaturated compounds, used as intermediates in organic synthesis, with application in pharmaceuticals.

Our research primarily focuses on developing novel heterogeneous catalysts. The immobilization of the nitrogen-based salts on support materials enhances their stability, ease of separation, and recyclability. Two inorganic porous materials were used as supports: mesoporous molecular sieve MCM-41 and the clay mineral montmorillonite. The materials were prepared by modification of the support surface with halogenopropyl trimethoxysilane, followed by quaternization of nitrogen compound. Various *N*-heterocycles were used as quaternization agents. The activity of prepared materials was evaluated in above mentioned reactions: the cycloaddition of carbon dioxide to styrene oxide and Knoevenagel condensation of benzaldehyde and malononitrile. The influence of the material structure on its catalytic activity was observed. The prepared materials demonstrated high efficiency in both reactions, producing styrene carbonate and benzylidenemalononitrile in high yields with 100% selectivity. This work provides insight into developing new effective catalysts, suggesting their application in green chemistry.

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Innovative Approach for Determining Basicity in Thermally Labile materials

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Layered double hydroxides (LDH) belong to the group of catalytic materials used in basic catalysis. Their basicity is the most important property for catalytic performance. Our work presents a possible method for the determination of such thermally labile materials´ basicity using liquid phase sorption of a specific probe. Anthranilic acid was chosen as an optimal probe, and two methods were used for measuring the basic site amount – HPLC-MS and DRUV-Vis. The chosen methods described exactly the behavior of the tested LDHs in the model reaction. The basicity of LDHs increased in the row LDH2 < LDH3 < LDH2.5 which was the same trend for the conversion of reactant achieved in a model reaction. The important parameter in the model reaction and in the basicity determination was the particle size of the materials. The amount of adsorbed anthranilic acid on LDHs was in the range 197.8 - 199.7 mg/g, which was ten times higher than the amount adsorbed on mixed oxides (MO, the precursor for LDH preparation, adsorbed amount of anthranilic acid 13.8 - 18.5 mg/g). The MO adsorption of anthranilic acid showed differences in overall basicity that were not visible under conventionally used method (temperature programmed desorption).The developed method seems to be promising in the determination of the basicity of especially thermally labile materials for which the conventional methods cannot be used[1].

References:

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Catalytic activity distribution of individual catalyst particles in one catalyst batch

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This work investigates inter-particle heterogeneity of the catalytic activity of hydrotalcite particles. Hydrotalcites are layered double hydroxides that exhibit basic active sites, which could vary in strength, and this variation could decrease reaction selectivity. While overall catalytic activity determination of the ensemble of catalyst particles is directly accessible by standard tests in a chemical reactor, catalytic activity determination of individual catalyst particles remains challenging. Here, we introduce a methodology for the chemical labeling of single hydrotalcite particles using a model reaction - base-catalyzed disproportionation of furfural. Furfuryl alcohol, one of the reaction products, could polymerize, and the polymerization products fluoresce. The higher the catalytic activity, the more reaction turnovers within the catalyst particle and the more intensive the particle fluorescence. Hence, fluorescence imaging of catalyst particles indirectly shows inter-particle variability in catalytic activity in this base-catalyzed reaction. This method reveals a variance of up to 20% from the mean fluorescence intensity. Therefore, the reaction rate determined in the catalytic reactor must have the same variance. This approach opens new doors for understanding the intricacies of catalytic activity and can pave the way for more effective catalysts.

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Chemical recycling of electro-waste by pyrolysis – monitoring of main chemical compounds in pyrolysis oil

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The chemical recycling techniques of waste materials are essential tools in modern applied research, providing valuable data for a better understanding of the circular economy as well as for other environmental topics. Pyrolysis, a thermal decomposition process in the absence of oxygen, is one of the attractive and effective ways of utilizing different types of waste. This chemical recycling technique converts waste, such as plastics and biomass, into various products, which are considered as alternative resources in the petroleum and chemical industry. Input raw material consists of liquid product of homogenized and pyrolytically transformed representative electro-waste (plastics from flat screens).
Pyrolysis oils are complex mixtures of numerous components and chemical compounds. After necessary sample pre-treatment techniques, a high-resolution qTOF analyzer in combination with gas chromatography was applied to perform detailed and robust non-targeted identification of compounds in pyrolysis oil. Presented results show various spectre of organic compounds, especially alkanes, alkenes, polyaromatic hydrocarbons, and heteroatomic molecules, consisting predominantly of O-bound / N-bound compounds and brominated/chlorinated substances. According to the particular content of heteroatomic molecules in liquid products, consequent after-treatment procedures should be applied, including adequate purification. A proper understanding of the pyrolysis of waste material and its mechanisms is a key aspect of the development of chemical recycling technologies. The presented study brings a deep insight into the topic of pyrolysis of complex plastic waste via the identification and discussion of groups of compounds that are formed during the pyrolysis process.

Recycling of polypropylene waste obtained from automotive industry

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Nowadays, plastics are an integral part of cars. While in 1970 there was only 40 kg of plastic in the car, nowadays it is up to 130 kg. The majority of plastics in cars are made of PP (35%). The remaining part consists of polyurethanes and polyvinyl chloride (total 35%), ABS, PA, PE and other types of plastics [1]. Plastic products in cars must meet strict criteria (e.g. quality requirements in terms of safety, heat resistance, etc.). Recyclates obtained from mechanical recycling are not suitable for their re-production due to inferior properties in comparison with original polymers. Therefore, much attention is paid to feedstock recycling. The benefit of feedstock recycling (thermal or catalytic cracking) is the production of chemicals, e.g. ethylene and propene, which can be reused for the production of polymers (plastics) meeting these strict criteria as well as fuels (gasoline, diesel). Of course, yields and composition of fractions depend on reaction conditions, type of reactor, residence time, and the presence or absence of a catalyst.

Considering the majority share of PP plastic in cars, our work is focused on the thermal and catalytic cracking of waste PP in a two-stage reaction system consisting of a batch semi-flow reactor and a flow reactor. The temperature on the bed of the catalyst located in the semi-flow reactor reached a temperature of 420°C. The weight of the input raw material was 25g and the ratio of catalyst to raw material varied in the proportions 1:14, 1:10 and 1:7. Both thermal and catalytic cracking were carried out under the same conditions and in the presence of nitrogen (60mg/min) as an inert. A thermal cracking experiment was used to compare and determine the effect of the catalyst on the composition and yields of gas and liquid fractions. 0.1 M acid-modified natural zeolite clinoptilolite was used in the catalytic cracking process.

Acknowledgement

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[1] https://www.plasticportal.sk/sk/progresivne-vyvijane-polymerne-kompozity-v-automotive/c/1945/

Substituted stilbenes in study of solid state fluorescence behavior dependence on carbazole position

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Substituted stilbenes with carbazolyl electron donor group, dicyanovinylene acceptor and a pair of side-aryls fluorescence both in solution ans solid-state. Polymorphism, regioisomerism and side-aryl engineering modifies the colour of intense solid-state fluorescence from yellow over orange and red, to deep red.

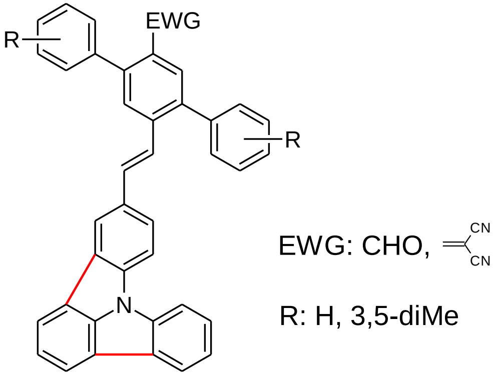

Figure 1: Syntheses of the compounds under study.

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Producing of 1,8-cineol from *α*-terpineol using heteropolyacid as catalyst

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Introduction

One of the many options, how to the utilize renewable resources, is the use of essential oils from plants that are rich on monoterpenes and monoterpenoids. α-Terpineol can be found, e.g., in lavender and leaves of conifer. It is signicantly used as a fragrance in soaps, perfumes, and cosmetics due to its lilac scent. Under acid catalyzed α-terpineol izomerization, we obtained a lot of products, the most interesting of them was 1,8-cineol.

Methods

Fumed silica and mesoporous silica MCM-41 were used as supports. Silicas were impregnated by a suitable heteropolyacid from water solution. The α-terpineol transformation was performed in a round bottom flask with a condenser heated in an oil bath on a magnetic stirrer under vigorous stirring. The samples without catalyst were diluted, and the composition was analyzed by GC-FID with a non-polar column. Compounds were identified using GC-MS.

Results

Firstly, we tested heteropolyacid in a homogenous arrangement. We obtained the best results using 0.5 mol.% of phosphotungstic acid. 1,8-Cineol was produced with selectivity 15-26 % in ethyl acetate. HPW was impregnated on fumed silica and MCM-41. Prepared heterogeneous catalysts were characterized and used in the reaction of α-terpineol in various green solvents (e.g., methyl acetate, dimethyl carbonate) for the study of the interaction between the heterogenous catalyst and solvent.

Conclusion

Based on heteropolyacids activity, HPW was chosen as a suitable for the impregnation of silica supports. 1,8-Cineol was produced with a selectivity higher up to 26 %. HPW was impregnated on fumed silica and MCM-41 in various contents. We studied the influence of the interaction between the heterogenous catalyst and solvent, especially green ones.

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Oil
Petrochemicals
Biofuels

Quality adjustment of liquid fractions from waste plastics pyrolysis and their use in the coprocess of hydrorefining

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Plastic waste with a high content of polyalkenes can be a valuable source of feedstock for refineries. In our research we developed a laboratory recycling unit consisting of a conical continuously operating reactor with a volume of 2 liters equipped with two heating zones. The mixture of waste polyethylene and polypropylene (1:1 wt) was pyrolyzed at 440 °C in the presence of carbon dioxide and the obtained pyrooil was further filtered and fractionated into four fractions - naphtha, kerosene, diesel, and residue. Impurities originating from additives and fillers from waste plastics also partially entered the pyrolysis oil. Detailed analysis of the distribution of impurities in individual fractions was performed. Material balance for pyrolysis in the conical reactor as well as yields of individual fractions after distillation were set. The diesel fraction was obtained with the highest yield in the amount of 33 wt%. The effectiveness of three different adsorbents - activated carbon, alumina, and silica gel was tested to capture impurities present in the diesel fraction. The coprocess of hydro-refining of kerosene and diesel fraction from waste plastics has also been carried out in the laboratory flow reactor in the mixture with fossil kerosene or vacuum gas oil (mixtures 1:9 V/V) at reaction conditions similar to the industrial hydro-refining units and in the presence of catalyst $NiMoP/\gamma\text{-}Al_2O_3$. Our result confirms the possibility of coprocessing of fractions from waste polyalkenes together with fossil fractions in a hydrorefining unit with no negative effect on the properties of the products.

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Vliv přídavku pyrolýzního oleje z použitých pneumatik na výtěžkovou strukturu produktů při fluidním katalytickém krakování

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Ve snaze omezit negativní klimatické dopady způsobené využíváním fosilních surovinových zdrojů pro výrobu paliv a chemikálií se hledají nové technologie pro jejich výrobu. Jednou z intenzivně sledovaných možností je přeměna polymerního odpadu na suroviny vhodné pro výrobu motorových paliv a petrochemie.

Bylo provedeno analytické vyhodnocení dostupného pyrolýzního oleje z použitých pneumatik. Tato data ukázala potenciální problémy při zpracování na jednotce fluidního katalytického krakování (FCC). Jedná se především o obsahy kovů působících jako katalytické jedy (Ni, V, Fe, Na), které jsou ve větším množství přítomny v pyrolýzních olejích. Dalšími ukazateli jsou obsah vázané vody, obsah sirných a dusíkatých látek a především obsah chloru, jehož limit je rafinérií přísně kontrolován.

Pyrolýzní olej z použitých pneumatik byl přidán do standardního ropného FCC nástřiku v množství 5, 10 a 20 hmotnostních procent. Takto připravené suroviny byly zpracovány na laboratorní jednotce ACE, která simuluje technologii FCC. Reakční teploty byly 500, 520 a 540 °C a tři dostupné rovnovážné FCC katalyzátory. Byla sledována celková konverze suroviny i celková výnosová struktura produktů. Zvyšující se obsah pyrolýzního oleje z pneumatik v nástřiku způsobil pokles celkové konverze z 3,0 % hmotn. na 6,5 % hmotn. Zároveň došlo také k výraznému omezení výroby žádaných produktů jako je propylen a benzinová frakce. Zvyšující se reakční teplota trochu zvýšila celkovou konverzi suroviny obsahující 20 % hmotn. pyrolýzního oleje z pneumatik. Z hlediska konstantní produkce koksu byla celková konverze vyšší o 0,6 % hmotn., zatímco produkce suchého plynu, propanu, propylenu, C_4 frakce a slurry vzrostla. Na druhé straně byl pozorován klesající trend u isobutanu, benzinové frakce a LCO frakce.

Identification of the impurities in the liquid products of thermal cracking of waste polyolefin blends and their separation

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There are also impurities present in the cracking products of waste polyolefins that could have a negative impact on their use in products or other downstream recycling technologies. Sources of impurities include catalytic system residues, functional additives, fillers, pigments and coatings. The subject of the research was the cracking of a mixture of waste PP blended with waste LDPE, the identification of impurities and the investigation of their effective elimination. Mechanically sheared fillers (TiO_2), halogen-containing compounds (Cl, Br) and polar compounds from the decomposition of prints and dyes were identified in the liquid cracking products. Filtration and high-temperature dehalogenation were used for their separation using two industrial adsorbents, Actisorb® Cl6 (Clariant) and AxTrap™ 858 (Axens). The waste PP contained 1.79 wt.% ash after annealing at 550°C. The major constituents were 2840 mg/kg Ti, 3656 mg/kg Ca, 489 mg/kg Al, 368 mg/kg Mg and 266 mg/kg chlorine. The bromine content was low below 0.1 mg/kg. The bulk of the fillers remain in the solid residue after thermal cracking. In the liquid fraction, the organic chlorine concentration was 206 mg/kg, the silicon content was 49.8 mg/kg, and the Al content was below 0.1 mg/kg. The tests were carried out in a tubular flow reactor with an adsorbent bed in the temperature range of 360-420°C in a CO_2 stream (0.2L/min). The high efficiency of both adsorbents was demonstrated. The dechlorination efficiency was 93-96 % (minimum organochlorine content was 0.38 mg/kg) and increased with increasing temperature. The desilication efficiency was also high 92-95%(the minimum value of Si content was 0.55 mg/kg. Secondary cracking of hydrocarbons with higher boiling points was carried out at 400 and 420°C. The degree of unsaturation increased and the end of the distillation curve decreased. In the gas fraction was dominated isobutene and propylene.

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Experience with the operation of new generations of pyrolysis heaters

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The pyrolysis section of ORLEN Unipetrol's steam cracker consists of eleven pyrolysis heaters. The type of the operated heaters changed significantly after an incident in 2015, when four of ten heaters were heavily damaged by fire. This part of the pyrolysis section was totally rebuilt in 2016 by T.EN. Due to the very positive experience with new heaters the last eleven one - identical to units built in 2016 was commissioned last year.

The recently operated pyrolysis section therefore offers a unique opportunity to compare the operation of three different designs of pyrolysis heaters - the original heaters equipped with SRT III reactors from the 70's, the revamped heaters from the beginning of the new millennium and up-to-date design represented by newly built heaters fitted with GK6 and SMK reactors arranged in three parallel rows.

Since the rebuilt of the pyrolysis section followed by the re-commissioning of the steam cracker in 2016, no comparison of the individual heater designs has been made, both in terms of the economics of operation and the achieved yield vectors. Such a comparison presented in this paper was made possible by a detailed analysis of operational data and also by the utilization of a hot cracked gas sampling method developed at ORLEN Unipetrol. The results obtained by the detailed analysis of the operational data and a comparison of the yield vectors are discussed focusing on the innovative technical solutions distinguishing the new pyrolysis heaters from the original ones.

The current increase of energy costs, emission fees as well as other operating costs make a constant pressure on the identification of ways how to reduce energy consumption and optimize assets operation. Thus the pyrolysis section consumes on average 60 percent of the total steam cracker energy consumption, any system improvement or better technical solution has a significant impact on the overall economy of plant operation. The results presented in this paper prove this goal was successfully achieved.

The use of multivariate statistics and mathematically modelled IR spectra for determination of HVO in diesel fuel

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Blends of diesel fuel with certain portion of bio-components are currently increasingly represented on the market. The most common bio-component for diesel engines is FAME (fatty acid methyl ester), but the share of diesel with HVO (hydrotreated vegetable oil) content has been increasing in recent years. HVO has many advantages in mixture with diesel, compared to FAME, but the fact remains that it is difficult to detect and quantify it in this mixture. The reason is the great similarity in the hydrocarbon composition of HVO and diesel fuel. A commonly used method for determining of HVO content is isotope C14 radioanalytical analysis, which can be performed by using LSC (liquid scintillation crystal) or AMS (accelerator mass spectrometry). However, the important fact is that both methods are very expensive. For this reason, the infrared spectroscopy followed by chemometric data processing was used for the HVO content quantification in the blends with diesel.

Infrared spectroscopy in ATR mode was utilized and 5 PLS prediction models were prepared. Standards used in these models consist of 10 different diesel fuels and 5 different HVO fuels. Calibration standards were created by mathematical combination of the spectra of the neat fuel components (HVO and diesel) with each other. The models were validated using standards consisting of both mathematically modelled spectra and real measured spectra . All 5 models were optimized for minimalization of prediction error. Mean centring and two smoothing techniques were used for the optimization.

Chemical Characterization of Pyrolysis Bio-oils from Cellulose, Hemicellulose, and Lignin

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Bio-oils from lignocellulosic biomass pyrolysis are promising renewable feedstock for producing oxygen-containing chemicals or advanced biofuels. A more widespread use of bio-oils requires more detailed knowledge of their composition. In this work, we prepared bio-oils by the pyrolysis of cellulose, hemicellulose and lignin (*i.e.*, main building blocks of lignocellulose). For the obtained bio-oils, we performed analyses of basic physical and chemical properties and a comprehensive chemical characterization also. The results obtained for these structurally less complex bio-oils can be helpful to understand the chemical composition of whole bio-oils in more detail.

EPOXIDATION OF METHYL ESTERS OF CAMELINA SATIVA OIL AS A SECOND-GENERATION BIOFUEL

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Current issue is searching for renewable sources for production of various materials or energy, which are currently 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 currently produced from crude oil.

The epoxidation of methyl esters of the non-edible Camelina sativa oil (second-generation biofuel) was carried out because it contains mainly unsaturated fatty acids, which are suitable for epoxidation. The novelty lays in the explanation of epoxidation process by the combination of statistical analysis and quantum chemistry thermodynamic calculations. The epoxidation can solve an increasing ester production, which arises together with increasing glycerol production by transesterification of vegetable oil. The composition of epoxidation products was checked in detail (GC-MS) at various reaction conditions including oil refinement. The mutual relations between them were statistically evaluated and mathematical models were constructed. According to the statistical analysis, the reaction time and temperature had the highest effect on the products' composition and oil refining is unnecessary. Moreover, the Raman spectroscopy was used to determine the iodine value, i.e., ester conversion without the use of chemicals. These outcomes will make the process of epoxidation of Camelina sativa more environmentally friendly.

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POTENTIAL OF HETEROGENEOUS CATALYSTS FOR ETHANOL VALORIZATION

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Ethanol stands out as one of the most promising chemicals for the production of sustainable derivatives like butadiene, ethylene, ethyl acetate, acetaldehyde, and butanol. Presently, ethanol is primarily derived from the fermentation process of sugar-based crops and lignocellulose biomass. It serves as a commonly used biofuel, often blended with gasoline at a rate of 10%. However, ethanol's high miscibility with water can lead to an increase in fuel water content during long-term storage. In contrast, butanol exhibits a lower affinity for water and boasts a higher energy content compared to ethanol. Its versatility extends to applications in the synthesis of butyl acrylate, butyl acetate, glycol ether, and as a direct solvent in textile and chemical processes, including plasticizer production. Moreover, the global butanol market is expected to grow by 6% from 2021 to 2031.

While butanol is traditionally produced through fermentation, it can also be synthesized from ethanol using the Guerbet reaction. This sequential process involves dehydrogenation, aldol condensation, and hydrogenation steps, each requiring specific catalysis. Redox catalysts, typically containing copper, facilitate the hydrogenation and dehydrogenation steps, while acid-based catalysts, commonly potassium or sodium hydroxides, drive the aldol condensation. Despite yielding not only butanol but also branched alcohols like 2-ethyl-butanol, the Guerbet reaction suffers from lower selectivity toward the desired product. Consequently, our research is directed toward developing optimized reaction pathways, including the exploration of suitable catalysts or catalyst groups and the examination of reaction conditions.

Our research methodology centers on the analysis of individual reaction components, necessitating varying reaction conditions. For instance, in the aldol condensation of acetaldehyde, we observed a higher selectivity toward crotonaldehyde. Subsequent hydrogenation of crotonaldehyde yielded butanol at 100°C. The aldol condensation reactions were conducted in stainless steel autoclaves, with rehydrated mixed oxides of Mg-Al demonstrating superior activity. Comparative studies with Mg-Al mixed oxides facilitated the determination of the optimal catalyst quantity.

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USE OF METHYLDICYCLOPENTADIENE FOR THE PRODUCTION OF RESINS

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The paper deals with the preparation and testing of modified resins based on the methyldicyclopentadiene (MDCPD) as a by-product in the production of dicyclopentadiene (DCPD). Different types of MDCPD-based resins were prepared from several different qualities of initial MDCPD and compared with DCPD-based resins and standard resins. Unsaturated polyester resins, alkyds and hydrocarbon resins were targeted. Formulations of the recipes were optimized in order to improve some properties of the prepared resins. On the basis of the tests carried out, it was confirmed that MDCPD can be used for the production of resins, which are capable of competing with standard and DCPD-based resins.

PYROLYSIS OF WASTE PLASTICS - HETEROATOM REMOVAL AND CHALLENGES

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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, are unable to 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, waste plastics contain numerous impurities that migrate into the pyrolysis oil [1], making them unsuitable for processing in the petrochemical industry due to exceeding heteroatom concentration thresholds.

Pyrolysis of model polymer blends (polyolefins with PA6, PUR, ABS) was performed to identify contaminating components, mainly nitrogen. These components were subsequently removed by adsorption during stepwise pyrolysis or by extraction from the resulting pyrolysis oil. It was found that the polar compounds were selectively removed, but non-polar compounds with heteroatoms remained in the pyrolysis oil. Despite promising results from literature reviews, these results were not confirmed by pyrolysis of model polymer blends in our lab.

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ASSESSMENT OF PROPANE-PROPYLENE FRACTION SEPARATION ALTERNATIVES

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Propylene holds a significant position in the petrochemical industry. Its global production increased from 84 million tons per year in 2013 to 120 million tons per year by 2022. Currently, its almost entire worldwide production is covered by two processes. Over 50% comes from steam cracking of hydrocarbons, and 35% is produced through fluid catalytic cracking. The technological processing of propylene imposes high demands on its qualitative parameters. High purity of propylene, equal to or greater than 99.5 wt.%, is required. This requirement places high demands on its separation. Propylene is obtained from a mixture of propane and propylene, both components have very close boiling points, making separation technologically and energetically demanding. Obtaining propylene by distillation requires a high reflux ratio and a large number of equilibrium stages. Due to their dimensions, these distillation columns rank among the tallest columns in practice, reaching heights exceeding 100 m. Currently, operating columns at a reduced pressure (10 bar) and utilizing a configuration with a heat pump is gaining prominence. Overhead vapors are compressed in a compressor and subsequently used for heating in the column's reboiler. This configuration combines the condenser and reboiler into a single unit, reducing the energy requirements of the process. A rigorously designed model of a column with and without a heat pump was constructed. These alternatives were compared in terms of economic, energy, and environmental aspects, revealing that the configuration with a heat pump is more advantageous. The constructed system was compared with real operational data, and very close parameter values were achieved.

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CORROSION PROPERTIES OF PYROLYSIS OILS FROM WASTE PLASTICS AND TYRES

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More than 400 000 tonnes of plastic waste are produced in the Czech Republic every year. Only 18% of this amount is recycled, less than 40% is recovered for energy use and the remaining plastic is landfilled. Pyrolysis is a promising way of processing this waste, producing pyrolysis oil, which can be used as a feedstock for the production of fuels and petrochemicals. However, this oil contains undesirable components such as halogens and other heteroatoms, olefins, water, etc. As a result, pyrolysis oils have low stability or are corrosive, which causes problems in transportation, storage and processing.

In the present work, corrosion tests of pyrolysis products of different types of waste plastics and waste tyre rubber were carried out on copper using modified ASTM D130 standard method and on steel coupons. At the same time, the change in oxidation stability of fresh pyrolysis oils and oils after corrosion tests was studied. The samples of oils obtained by tyre pyrolysis showed higher corrosion effects on steel. Comparison of the results of the oxidation stability of pyrolysis oils before and after corrosion tests shows, among other things, that the presence of copper shortens the induction time for some pyrolysis oils from waste plastics by up to ten times. This demonstrates a significant change in the properties of pyrolysis products after contact with construction materials.

EXPLORATION OF THE ENVIRONMENTAL LOAD AT HOREHRONIE IN THE VILLAGE PREDAJNÁ

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One of the priorities of the Government of the Slovakia in the area of the environment is also the removal of environmental loads (ELs), which pose a danger to human health, the environment, and increase the contamination of soil, rock environment and groundwater. Gudron pits at Horehronie are among the largest ELs in Slovakia, while the largest of them is located in the cadastral territory of the village Predajná. Due to the fact that ELs - landfill Predajná I and Predajná II are locations with a high priority, their rehabilitation is highly desirable and necessary. Both gudron landfills are located in a geologically and hydrogeologically unsuitable environment with a high permeability of krastic carbonate rocks.

The subject of the work was the analysis of pasty and solid gudron samples. The results of the analysis show that they contain a high proportion of water, inorganic salts and secondary pollution. After extraction and dewatering at ambient temperature the water content can be radically reduced. Energy use of tars treated in this way is possible as one alternative, respecting the high content of total sulfur, highly corrosive components of flue gases and neutralization of free sulfuric acid with CaO. Tars can be neutralized by mixing with CaO. It is technologically advantageous to use aromatic fractions during neutralization for better contact of CaO with tars. A beneficial side effect is an increase in calorific value. For the chemical use of tars, it is necessary to separate the organic part from the inorganic part. Extraction with a mixture of aromatic and polar solvents proved to be advantageous.

These results of the analysis will serve for the needs of developing a feasibility study, as well as input data for the project to rehabilitate this environmental load.

The rehabilitation of the ELs in the village Predajná will be carried out in accordance with the measures resulting from the State Program for the Rehabilitation of the ELs (2022-2027), while it will be a significant contribution to the improvement of the environment in the area of Horehronie.

Rheological and frictional behavior of Environmentally Acceptable Lubricants for maritime applications

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Introduction

To reduce the environmental pollution, sea waters in particular, the environmentally acceptable lubricants (EALs) should replace mineral oils at all sea water-oil interfaces as required by several national legislation rules (VGP 2013, Polar Code 2017). In contrast to mineral oils the EALs must meet environmental criteria. Besides the excellent lubricating parameters and stability, they must meet strict criteria for biodegradability, biotoxicity and bioaccumulation. The fact that these criteria sometimes counteract against each other, for example long lifetime vs. high biodegradability, the task for EAL lubricant formulators became very difficult. Therefore, the lubricating properties of newly formulated EALs have to be carefully investigated in parallel to their environmental characteristics. The task for EAL formulator to prepare lubricant for the targeted application includes careful selection of a base fluid in combination with additive or additive packages that have to be mutually compatible under wide range of operating conditions.

Methodology

In this contribution we investigated rheological and frictional behavior of several synthetic ester base fluids without and with additives as EALs candidates for maritime applications. The rheological and frictional properties were characterized by HAAKE-MARS 60 rheometer with co-centric cylinder geometries and tribology measuring cell for frictional properties characterization.

Results

The tested samples of EALs and their base-fluids were compared with their mineral oil-based counterparts and commercial EALs of the same viscosity grade. We concluded, that the newly formulated EALs are fully competitive with their mineral oil-based predecessors in terms of performance while being environmentally acceptable.

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Inorganic technology

ZEOLITES IN FERTILIZERS

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Natural zeolite - clinoptilolite is a hydrous aluminosilicate of cations of alkali metals and alkaline earth metals from the heulandite group, which have the ability to exchange their exchangeable cations for others. The three-dimensional lattice of zeolites generally contains holes forming channels in which cations or molecules, for example water, are adsorbed[1].

The multidirectional use of zeolites in agriculture results primarily from their high porosity, sorption-ion-exchange capacity and well-developed specific surface area. Their direct application to the soil not only has a beneficial effect on the soil sorption capacity, but also reduces soil acidification and increases the efficiency of nutrient use. Better utilisation of nutrients from fertilisers gives higher yields and reduces nutrient dispersion in the environment[2].

Zeolite as an additive to ammonium nitrate affects the phase transition temperature of crystal modification IV, which is a stable form for storage. A typical phase transition temperature of IV-III is 32 to 34 °C[3]. Modified ammonium nitrate have a higher transition temperature, depending on humidity, preparation method and the presence of additives.

Each phase transition causes the degradation of granular fertilizer reduces mechanical strength, increases the dust and hydrophilicity.

The contribution is devoted to the research of granular ammonium nitrate fertilizer with zeolite. The raw material is zeolite - clinoptilolite from Nižný Hrabovec in the east of Slovakia, mined by Zeocem a.s. Bystré.

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PHOSPHATE ASH AS AN ALTERNATIVE WASTE SOURCE OF PHOSPHORUS FOR FERTILIZER PRODUCTION

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Production of fertilizers containing phosphorus often involves processing phosphates from phosphate rock. Phosphate rock is a natural source of phosphorus, a crucial nutrient for plant growth.

In 2014, the EU classified phosphate rock as a critical raw material, and in 2017, phosphorus as an element was added to the list[1,2]. Typical phosphate rock contains phosphate expressed as P_2O_5 at a concentration of 25 – 40%.

The extraction of phosphorus from waste sources is gaining increasing attention because phosphate rock resources are depleting. One alternative waste source of P is ash from sewage sludge after thermal treatment. Phosphate ash contains phosphorus compounds that can be biologically utilized by plants. The phosphorus content, expressed as P_2O_5, in sewage sludge ash can range from 6 – 25%[3]. Phosphate ash is also enriched with other nutrient components such as Ca, Mg, and possibly K. The exact composition of phosphate ash may vary depending on the specific production process and raw materials used.

Industrial technologies using sewage sludge ash as a raw material demonstrate high efficiency and utilization with a lower environmental impact. Raw phosphate ash is often processed into fertilizers or can be used as an industrial additive to improve soil properties.

This contribution describes the direct application of phosphate ash after thermal processing of sewage sludge in the production of granulated fertilizers, considering not only nutrient content but also heavy metals in accordance with EC regulation[4].

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Crystallization kinetics of Al_2O_3-Yb_2O_3-Er_2O_3 glasses

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Aluminate glasses possess unique physical and chemical properties, making them highly durable materials for challenging conditions such as high temperatures and corrosive environments. The addition of rare earth oxides RE_2O_3 to alumina-rich systems can further enhance their properties. However, their wide utilization is greatly influenced by the preparation conditions, which require high melting temperatures and high cooling rates. Precise studies of their thermal behaviour, and crystallization in particular, are necessary to understand and develop conditions for efficient preparation of glass or glass ceramics with this composition.

This work focuses on Al_2O_3-Yb_2O_3-Er_2O_3 glasses ($62.5Al_2O_3 \cdot (37.5 - x)Yb_2O_3 \cdot xEr_2O_3$, x = 1, 3, 5) – their preparation and thermal behaviour. The samples were prepared by the combination of the Pechini sol-gel method and flame synthesis. The study of thermal behaviour was carried out by differential scanning calorimetry (DSC) and supported by scanning electron microscopy (SEM) and X-ray powder diffraction (XRD). Thermal analyses were performed in the temperature interval of 30 – 1100 °C under non-isothermal conditions with the heating rates of 0.25, 0.5, 0.75, 1 or 1.25 $°C.min^{-1}$ and also under isothermal conditions at 914 °C for 90 min. Kinetic parameters – activation energy E_A, frequency factor A and Avrami exponent n were calculated by the JMAK model. The results of SEM, XRD and kinetic analysis confirmed the chemical reaction-controlled crystallization process with linear time dependence of nucleation rate and 2-D (5.0 mol.% Er_2O_3) and 3-D (1.0 and 3.0 mol.% Er_2O_3) growth of cubic YbAG.

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Composites based on phase change materials for heat energy storage

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An inability to reduce the consumption of natural raw materials together with the discrepancy between the supply and demand of energy from renewable sources leads to the request for long-term energy storage. Phase change materials (PCMs) seems to be siutable candidates for this task, and several salt hydrates have been explored intensively. However, large-scale implementation of PCMs into the energy system is still lacking and requires significant improvement of the proposed PCMs. The main demands of PCM are: low price, non-toxicity and its stability over thousands of phase change cycles. In the case of phase change cycles (including melting – crystallization in the case of salt hydrates) there are three main aspects negatively influencing its repeatability and stability – phase separation, supercooling, and low thermal conductivity. Phase separation can obviously be overcome by encapsulation or the addition of filler. Supercooling, i.e. the temperature of the phase change during the charging being higher than that of discharging, can be suppressed by the addition of nucleating agent. In addition, the improvement of the thermal conductivity can be done by encapsulation or by the addition of better thermal conducting material into the PCMs. However, if we solve each of these aspects separately by adding other substances, the PCM content in the composite will be reduced so much that we will only get a small amount of stored heat. For selected salt hydrates, nucleating agents were tested to suppress supercooling but also to increase thermal conductivity. At the same time, attention is also paid to phase separation. The effects of individual added substances on the total amount of accumulated heat and on the stability of these composites for long-term use are discussed in detail.

An experimental study of corrosion of metals used for latent heat storage

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The lack of fossil fuels and their negative impact on the environment has led to the search of alternative options in recent years. One of such options is the use of solar energy to generate heat. There are mainly two types of thermal energy storage (TES) systems, sensible storage systems and latent storage systems. Over the past decades, substances able to store heat in the phase change have been extensively studied. These substances are called phase change materials (PCMs) and their ability to accumulate heat is significantly higher than that of substances utilising sensible heat. Thanks to their feature accept or deliver heat at a constant temperature they have found application in many applications.

Extensive research has been carried out in the identification of various PCMs in a wide range of phase transition temperature and heat of fusion. The most important group of PCMs are inorganic salt hydrates due to their latent heat of fusion (86-328 kJ/kg), higher thermal conductivity and lower price compared to paraffins. Among their disadvantages belongs incongruent melting of the most hydrates and significant supercooling and corrosive effects on the metallic components of the storage device. To apply these materials in the latent heat storage systems, it is necessary to know their corrosion effect on the construction materials.

In this work, corrosion behaviour of selected metals used in heat exchangers (stainless steel, carbon steel, aluminium) was studied in assumed PCMs. Corrosion sensitivity of selected metals was assessed through electrochemical measurements and gravimetric analysis.

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Použitie EIS na charakterizáciu modifikovaných tanátových vrstiev

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Úvod

Elektrochemická impedančná spektroskopia (EIS) je metóda užitočná pri monitorovaní korózie a ochrany pred koróziou. Pri vhodne zvolenom rozsahu použitých meracích frekvencií sa považuje za nedeštruktívnu techniku, ktorá napomáha v utvorení obrazu o koróznej odolnosti študovaných povlakov. Jedným z typov povlakov, ktoré sa používajú na ochranu železných predmetov pred koróziou sú konverzné povlaky na báze prírodného tanínu. Výsledná tanátová vrstva na povrchu predmetu – tanát železitý neposkytuje dostatočnú odolnosť voči korózii v prostrediach s vyššou vlhkosťou. Modifikovaná tanátová vrstva s hydrotalkitom má prispieť ku zvýšeniu koróznej odolnosti.

Metodika

Tanátový konverzný povlak sa nanášal technikou ponoru. Po predúpravných operáciách sa povlak aplikoval v dvoch vrstvách. Pripravené vzorky sa charakterizovali pomocou EDX, SEM a EIS techník. Elektrochemické charakteristiky sa získali v ASTM elektrolyte po stabilizácii OCP po dobu 40 min s trojelektródovým zapojením: nasýtená kalomelová elektróda – RE; grafitová elektróda – CE a vzorka s rozmermi 1x1cm^2 – WE [ASTM D1384-87 solution]. Po ustálení OCP sa EIS sa meria ako striedavá zložka prúdovej odozvy voči OCP pri amplitúde 20 mV s rozsahom frekvencií 10^{-2} – 10^5 Hz.

Výsledky

Porovnaním Nyquistových a Bodeho diagramov je pozorovaný posun kriviek spôsobený modifikáciou tanátového povlaku. Na základe fitovania jednotlivých kriviek je zhodnotený vplyv účinku hydrotalkitov na kvalitu modifikovaného tanátového povlaku.

Záver

Na základe meraní sa zistilo, že modifikovaný tanátový povlak prispieva ku zmene elektrochemických charakteristík v sledovanom elektrolyte než čistý tanátový povlak. EIS je tak vhodnou elektrochemickou technikou na charakterizáciu modifikovaných tanátových povlakov.

Táto práca vznikla vďaka podpore MŠVVaŠ SR v rámci projektu VEGA 1/0747/21.

Possibility of underground hydrogen storage in the Czech Republic

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Development of hydrogen technologies is strongly depend on the accessibility of sources of hydrogen the Czech Republic. Sources for production of green hydrogen are strongly limited. Solar energy is available only for limited part of day. Potential of wind energy is limited by inland character od republic without high mountains and with many limitations like natural parks, bird protective areas, human settlements and etc. Potential of renewable sources, which are necessary for green hydrogen production is insufficient for basic supply of electric energy for most of the year. Green hydrogen will have to be imported from areas with better conditions for renewable sources. Three areas are potential available for Czech Republic. North sea and west of Ukraine with wind farms. North Africa with solar plants. Hydrogen from these areas will be transported into central Europe by exist or new pipelines. The pipelines form a dense network with many parallel lines. Line with possibility of store transported medium is preferred. Storing is important for balancing consumption differences between summer and winter. Overproduction of renewable sources is limited into few months in year and this energy have to be stored for more than three months for winter time. If we want store this energy overproduction into hydrogen, we need storage for hydrogen. Capacity of classical gas tanks is insufficient. This is reason, why we need to build new underground hydrogen storage or convert exist underground storage for nature gas to hydrogen. Storing of hydrogen has some specific problems compared to storage of natural gas. Without solving these problems will be import of green hydrogen into Czech Republic impossible. It will be problematique for many industries like ammonia production, food processing, metal production, glass production and etc.

Modelling of Hydrogen Production for Hydrogen Mobility: A Comparison of Renewable Sources of Energy

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Hydrogen can be used in a large variety of technologies including various types of industry. Currently, hydrogen mobility is gaining attention. In hydrogen mobility, the hydrogen is consumed in hydrogen fuel cells resulting in electrical energy and pure water. To achieve zero-emission hydrogen mobility, the hydrogen must be produced without CO_2 emissions – from renewable sources of energy by water electrolysis.

Renewable sources of energy (RSE) produce electricity in an unstable and (mostly) unpredictable manner. Therefore, mathematical modelling must be used to calculate the hydrogen production. A mathematical model was created, which can, from the known data of RSE power output, estimate the amount of hydrogen produced.

This model can be used to assess the viability of different RSEs and their combinations as the power supply of the water electrolyser. The intended use is to find an optimal size of an electrolyser to a given unstable power-source capacity to achieve highest hydrogen production with low investment. Furthermore, the production data can be used to assess a need for hydrogen storage, as a stable hydrogen supply needs to be maintained. The results from the model involve run-time statistics and also CAPEX estimates. The CAPEX estimates together with the predicted hydrogen production can be used to assess the return on investment.

Tools such as the presented model are crucial in the strategic planning of hydrogen based public transport.

This project is financed by the Technology Agency of the Czech Republic under grant TO01000324, in the frame of the KAPPA programme, with funding from EEA Grants and Norway Grants.

Influence of the Preparation Method on Performance of NiFe Layered Double Hydroxides for Oxygen Evolution in an Alkaline Environment

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Hydrogen is considered a promising alternative to unsustainable fossil fuels as it has great potential as an energy carrier. One of the reasons is that hydrogen can be produced from water by electrolysis using renewable energy. Among electrolysis technologies, alkaline water electrolysis (AWE) offers low-cost characteristics because it uses non-precious catalysts and inexpensive construction materials. However, sluggish kinetic of oxygen evolution reaction (OER) represents a limitation of the AWE. Therefore, the development of a stable, inexpensive electrocatalyst with high activity to OER is still highly demanded.

Many non-precious metal-based catalysts show low overpotential towards OER, and thus attract tremendous research interest. A wide range of OER catalysts based on Mn, Fe, Co or Ni metals have been reported. These catalysts are prepared in various forms, for example, oxides, (oxy)hydroxides, phosphides, nitrides, or selenides. Among these, NiFe layered double hydroxides (LDHs) showed lowest overpotential for OER.

The aim of this work is to prepare NiFe LDHs catalyst by different methods and, based on the performance of the catalysts, choose the most appropriate method. In the next step the preparation method will be optimised, and the influence of intensified process on the properties of the catalyst verified.

Solvothermal, electrodeposition and precipitation methods will be used. The catalysts will be characterized using linear sweep voltammetry on rotating disc electrode, XRD and SEM-EDS. Electrochemical impedance spectroscopy will be used to measure catalyst powder conductivity.

The results indicate that the properties of the catalyst, especially the electric conductivity depend on the preparation method as well as on the concentration of the salts in the deposition solution.

Acknowledgment

Financial support of this research by the Technological Agency of the Czech Republic under the project No TK02030103 “Research and development of a reversible alkaline fuel cell” is gratefully acknowledged.

Air Purification System for Fuel Cell Power Generators

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Intensive development of fuel cells in recent years has brought this technology to real applications such as cars, stationary power units, and backup devices. Despite several benefits of fuel cell technology, the quality of input gases requires precise pre-treatment. While the quality of hydrogen is guaranteed by its production process, the air is drawn from the open atmosphere. Air contaminants, including dust and raindrops, must be filtered out from the air feed into the fuel cell stack. Larger mechanical contamination is separated by a cyclone. Finer dust and pollen are captured by a fine HEPA filter. Periodic filter cleaning is necessary to keep the HEPA filter efficient. Whereas backflow is used in stationary applications, vibrations provide cleaning effect in mobile applications. Since mechanical filters were originally designed for combustion engines, their flow rates range is currently not optimised for fuel cell applications. Nevertheless, despite lower flows than designed, mechanical cyclone-based separators from automotive applications fulfil the requirements for fuel cells.

A critical aspect of air filtration is the elimination of chemical contamination. It is caused by external factors such as industrial activities, intensive traffic etc. A special filter layer based on activated carbon is used to capture corresponding pollutants such as organic vapours, ammonia, or sulphur compounds. The efficiency of air filtration has been studied alongside the influence of impurities on the function of PEM fuel cells.

A sorption filter is capable of eliminating peak contamination and thus preventing the poisoning of the fuel cell. Low concentrations of organic or ammonia contaminants do not lead to a visible decrease in fuel cell performance. The critical parameter for chemical filter application is, however, its sorption capacity. Therefore, the determination of filter lifetime is crucial for the proper functioning of fuel cell systems.

This work was supported by the Technology Agency of the Czech Republic under project no. TK050200013.

Fuel Cell's Metallic Bipolar Plates – Advantages and Challenges

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Nowadays, an increasing pressure on the transition from traditional fossil fuels-based energy sources to the more efficient and less polluting alternatives calls for changing established approaches. In this particular contribution, we will focus on the proton exchange membrane fuel cells (PEM FCs) as an alternative energy source fulfilling the above requirements. Heavy weight and low production capacity of the fuel cells stacks are some of the obstacles deteriorating broad spreading of this technology. One of the reasons for this are that bipolar plates. They represent most bulky component of the fuel cells stack and at the same time contribute most significantly to the total weight of the unit. Utilization of metallic bipolar plates offers a solution to this problem, together with improved electric and heat conductivity in comparison with other composite or carbon-based materials. Mechanical properties of the metals allow to use very thin foils (typically 0.1 mm) with suitable profiling as a basic material for the bipolar plate production. Mechanical properties also affect the methods of metallic bipolar plates production. As typical production methods examples, embossing or hydroforming may be mentioned here. These represent well-established, high production capacity industrial technologies.

The above approach, however, brings about some issues. The first one is the danger of the MEA poisoning by the bipolar plate corrosion products. The second one is connected to the shape of the reactant distribution channels originating from the method of their production and mechanical properties of the metal sheet.

First of the above-mentioned issues is currently solved by a costly surface treatment. The current study is addressing an alternative approach utilizing a polymeric film filled with aligned electrically conductive particles. The issue of the distribution channels geometry is solved by means of the mathematical modelling allowing for a targeted parametric study.

The aim of this contribution is to present the results achieved in the direction of an alternative treatment of the metallic bipolar plates and of a deeper understanding of the flow field geometry on the mass and charge transport limitations in an operating PEM FC.

The CORE project Nr. TO01000306 benefits from Norway and Technology Agency of the Czech Republic Grant within the KAPPA Programme.

Composite membranes for CO_2 separation based on PIM-1

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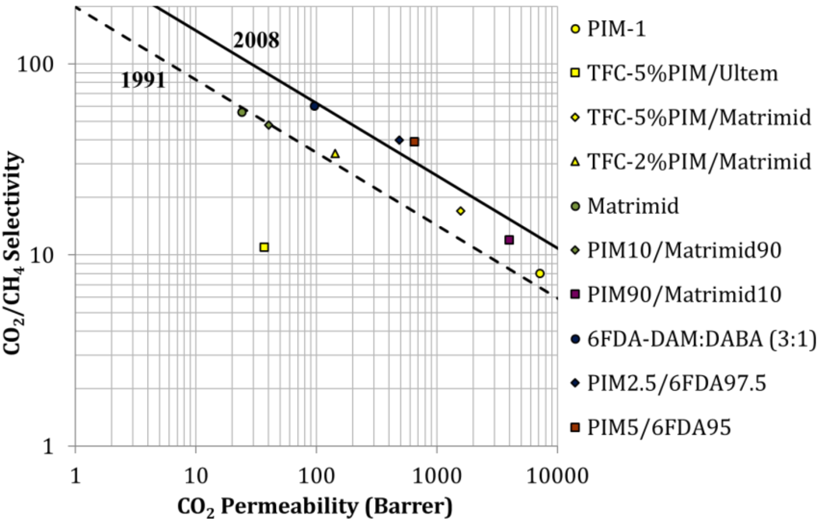
Membrane gas separation presents an alternative technology to the traditional gas separation processes. Polymers of intrinsic microporosity (PIMs) exhibit high CO_2 permeability and moderate CO_2/CH_4 selectivity. The main disadvantage of PIM-1 is its relatively high price. The preparation of PIM-1-based composite membranes presents an opportunity to reduce the amount of PIM-1 used per unit area of the membrane and improve the gas separation performance.

The different approaches reducing the PIM-1 amount per unit membrane area have been tested in this work. The novel i) blended dense PIM-1/Matrimid®5128 and PIM-1/6FDA-DAM:DABA (3:1) membranes, and ii) thin-film composite membranes composed of cross-linked Matrimid®5128 or Ultem®1000 porous support and PIM-1 layer were synthetized. The gas separation performance and stability of prepared membranes were evaluated at several feed pressures using binary CO_2/CH_4 1:1 feed mixture. Moreover, the FTIR, SEM, TGA and DSC methods have been used for membrane characterization.

The addition of PIM-1 in 6FDA-DAM:DABA (3:1) provides outstanding CO_2/CH_4 separation results. The introduction of low PIM-1 loadings brings an important increase of mixed-gas permeability without losing the separation factor. The performance of these membranes surpasses the Robeson limit and introduce a perspective material for application in biogas purification.


2008
1991
100
10
1
1
10
100
1000
10000
CO2/CH4 Selectivity
CO2 Permeability (Barrer)
PIM-1
TFC-5%PIM/Ultem
TFC-5%PIM/Matrimid
TFC-2%PIM/Matrimid
Matrimid
PIM10/Matrimid90
PIM90/Matrimid10
6FDA-DAM:DABA (3:1)
PIM2.5/6FDA97.5
PIM5/6FDA95

Effect of lime source on crystallisation of anorthite in ceramic production

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Ceramic products with a calcium component are an integral part of construction materials, especially for interior use. Ceramic tiles provide resistance to moisture, provide noise regulation, facilitate surface cleaning, etc. Functional and design requirements, which represent new challenges for ceramic technology, are claimed on this type of ceramic product. Complying with the current trend of large-format tiles with dimensions that can reach up to 1.5 x 3 m in extreme cases is quite challenging. It is necessary to ensure that the ceramic body is not deformed and that the dimensional tolerance established by the standard, which varies between 0.5 and 2%, is maintained. For these reasons, the work was focused on the Al_2O_3-SiO_2-CaO ceramic system, which represents a promising way to maintain dimensional standards in the case of an optimal design of the ceramic body.

Anorthite is the main crystalline phase formed during firing, which provides the dimensional stability of the products. Deformation of large products due to the delay in shrinkage in the temperature range of 950-1100 °C could be prevented by a well-designed ceramic body with an optimal part of anorthite. Considering that the temperature profile of the firing in industrial kiln changes relatively quickly in the area of maximum temperatures, this delay is very significant. For this reason, the work is focused on the study of the influence of different sources of lime on the crystallisation of anorthite. The effects of raw materials and firing conditions on the formation of the anorthite ($CaAl_2Si_2O_8$) phase were investigated using differential thermal analysis (DTA) – thermogravimetry (TG) and powder X-ray diffraction (XRD).

Study of the Conversion Reaction of Sodium Perchlorate and Ammonium Chloride

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Chloristan amonný je v současnosti velice žádaným produktem, používá se zejména jako hlavní složka pevných raketových paliv. Pro přípravu čistého chloristanu amonného je zásadní reakce chlorečnanu sodného s chloridem amonným (nebo kyselinou chlorovodíkovou a amoniakem) za vzniku produktů a to chloridu sodného a chloristanu amonného. Vše probíhá ve vodném prostředí a pro co nejdokonalejší oddělení produktů je nutná znalost rozpustností směsi chloridu sodného, chloristanu amonného a vody. Rozpustnosti čistých složek (NaCl a NH_4ClO_4) ve vodě jsou známy a tabelovány. Problém nastává u směsi chloridu sodného, chloristanu amonného a vody, protože může docházet k ovlivnění rozpustnosti jedné složky složkou druhou. V literatuře byl nalezen pouze jeden diagram rozpustnosti této směsi, a tento diagram se neustále, v různých formách, opakuje v literárních rešerších. Tento diagram vzájemné rozpustnosti byl publikován již v roce 1961 v časopise Chemical Engineering Progress [1]. Pro ověření tohoto diagramu byla provedena série experimentů rozpustností směsi chlorid sodný + chloristan amonný + voda. Při bližším pohledu na získané výsledky je patrné, že NH_4ClO_4 je nejméně rozpustný ze všech možných produktů při nízké teplotě, tedy se bude vylučovat jako první. Ovšem, pokud budou roztoky příliš koncentrované, začne krystalizovat i NaCl. Pro maximální výtěžek chloristanu amonného je tedy nutné mít koncentraci (rozpustnost) NaCl těsně pod bodem nasycení při technologicky co možná nejnižší teplotě.

Literatura:
[1] Chemical Engineering Progress (Vol. 57, No. 11, page 138 (Nov. 1961)).

Efektívna príprava železanu elektrolýzou

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Úvod

Železany sú zlúčeniny železa s kyslíkom v oxidačnom stupni +VI. Ide o takzvané „zelené“ oxidanty, ktoré sú vhodné na dočisťovanie odpadových vôd. V odpadových vodách sa nachádzajú rôzne škodlivé látky, ktoré železany vedia zoxidovať. Sú to napríklad antibiotiká, zvyšky liekov alebo hormóny. Z hľadiska ekonomiky sa železany radia k drahšej chemikálii, ale jej cenu vyvažuje jej veľká účinnosť a širokospektrálne využitie. Problémom môže byť aj ich stabilita, ktorá úzko súvisí s čistotou produktu, ktorý vieme pripraviť v tuhom stave. V našom výskume sa zaoberáme elektrochemickou výrobou železanu draselného a optimalizáciou celého výrobného procesu. Cieľom bolo preskúmať ako vplývajú rôzne parametre na účinnosť tvorby železanov, konkrétne sme sa venovali vplyvu teploty a prúdovej hustoty na zliatiny s rôznym zložením.

Metodika

V prvom kroku sme si pripravili zliatiny železa s prímesou legujúcich prvkov. Vyrobili sme ich tavbou v indukčnej peci a následným odliatím do valcových foriem. Ako legujúce prvky sme použili kremík a hliník. Ďalším krokom bola elektrolýza v roztoku hydroxidu sodného. Doba elektrolýzy bola 10 hodín a každú hodinu sme odoberali vzorku anolytu a analyzovali sme obsah železanu spektrofotometricky pri vlnovej dĺžke 500 nm. Experimenty sme vykonávali pri teplotách 20 a 30 °C a prúdových hustotách 40 a 80 mA cm^{-2}.

Výsledky

Získané výsledky preukázali, že pri nižšej teplote je prúdová účinnosť nižšia, lebo anóda nie je dostatočne aktivovaná na tvorbu železanov. Pri vyššej prúdovej hustote sa maximálna koncentrácia železanov dosiahne skôr, ale prúdová účinnosť je nižšia, čo je nevýhodné pre výrobu.

Záver

Je žiadúce pracovať pri podmienkach, ktoré vedú k najlepšej efektivite výroby železanov, a preto sa snažíme optimalizovať celý proces výroby, ktorý zahŕňa aj úpravu rôznych parametrov ovplyvňujúcich výrobu železanov. Z tohto experimentu vyplýva, že najvýhodnejšie podmienky pre zliatinu, pri ktorej dosahujeme vo všeobecnosti najlepšie výsledky sú: pracovná teplota 30 °C a prúdová hustota 40 mA cm^{-2}.

Poďakovanie

Táto práca vznikla s podporou grantových schém MŠVVaM SR prostredníctvom projektu VEGA 1/0436/23.

Chemical Processes and Devices

Glatt Ingenieurtechnik GmbH – From your product idea to industrial production

Buchheim J.[1], Vockenberg T.[1]

[1]*Glatt Ingenieurtechnik GmbH, Weimar, Germany*

Glatt Ingenieurtechnik GmbH – From your product idea to industrial production

As the world's leading expert in fluidized and spouted bed technology, GIT offers particle design and plant manufacturing from a single source. For functional powders, granules and pellets in food, feed and fine chemicals, our technology center is available to customers for their product and process development with reactor systems of various sizes. In addition to standard drying, agglomeration, functionalization or coating processes, reactions can also be carried out with solvent-based formulations under inert gas.

Based on many years of expertise in the field of process engineering and plant technology, we also manufacture customized fluidized bed reactors for special applications and even CVD processes in fluidized beds. There are no limits to the applied temperature range up to 900°C. Reactive gases can also be considered here.

From 50 nm to 50 µm: drying, coating and calcination in just one process step: Produce powder materials with new, previously unattained properties in the pulsating hot gas stream of the patented Glatt powder synthesis. Thanks to the particularly homogeneous thermal treatment up to 1.300 °C, ultra-fine powders produced this way are free of hotspots, easily dispersible and free of undesirable hard aggregates. Benefit from very high heat and mass transfer rates in the reactor and from the ability to specifically determine the layer thickness, porosity and activity profiles of your powder particles. You have full flexibility to adjust the chemical composition of your powders, achieve extremely good homogeneity and a narrow particle size distribution. The continuous process is easily scalable to industrial applications.

The contribution reflects the technological expertise of Glatt Ingenieurtechnik GmbH. Our powder synthesis will be highlighted in an oral presentation using selected examples.

DEVELOPMENT OF AN AUTOMATED MOLTEN SALT REGENERATION SYSTEM FOR CARBON NANOMATERIALS AND GRAPHITE SYNTHESIS

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[1]Slovak University of Technology in Bratislava, Faculty of Mechanical Engineering, Institute of Process Engineering, Bratislava, Slovakia
[2]Inegi, Porto, Portugal
[3]Universitat de Lleida, GREiA Research Group, Lleida, Spain
[4]UP Catalyst, Tallinn, Estonia

This work describes the design, construction, and implementation of an innovative molten salt regeneration system within the MoReCCU project. The system integrates with the UP Catalyst carbon nanomaterials and graphite synthesis reactors. The automated regeneration process removes solid products and impurities from the electrolyte mixture, enabling the sustainable production of high-quality carbon. Molten salt regeneration offers an environmentally friendly alternative to salt mining, while simultaneously enhancing crucial production factors like energy efficiency.

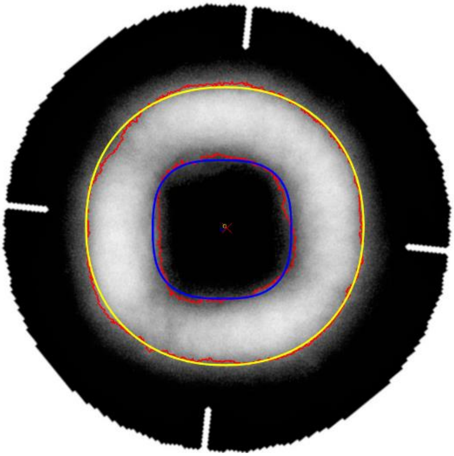
Acknowledgments:
This publication was created on the basis of the project Molten salt regeneration for carbon capture and utilization (MoReCCU, id: 23249) supported by EIT Manufacturing. The authors wish to acknowledge the Ministry of Education, Research, Development and Youth of the Slovak Republic by grant KEGA 003STU-4/2023.

Improved visual analysis of patterns forming on the bottom of a mixed tank when reaching suspension in a solid-liquid system by experiment and lattice Boltzmann simulation

Ing. F. Randák, Prof. Ing. Tomáš Jirout, Ph.D.

Czech Technical University in Prague, Department of Process Engineering

Mixing of solid-liquid systems is a common process in chemical engineering. Main effort is to reach full suspension of particles for optimal process conditions with the lowest possible mixing speed. A simple way to analyse reaching suspension is to measure the growing size of the ring that's being washed out in the bottom unsuspended particle layer of a transparent tank as mixing speed increases. A flat-bottomed transparent tank with $D = 0.3\ \mathrm{m}$ and four baffles was filled with water and spherical glass particles of $d_p = 484\ \mu\mathrm{m}$ to various concentrations, mixed by 6-blade PBT with $d = 0.1\ \mathrm{m}$. For each measured mixing speed below suspension, 30 images of the tank bottom patterns were taken in one minute. The images were then time-averaged and relevant shape boundaries were extracted in MATLAB. It was found that these boundaries are best fitted not with Euclidean circles, but with p-norm unit circles $r^p = x^p + y^p; p \in \langle 1; \infty)$, sometimes called Lamé curves. The experiment is then reproduced as lattice Boltzmann simulation in M-Star for comparison. For each case, the washed-out ring was assigned mean inner and outer radii as well as p values describing its 'rectangularity' bestowed upon the otherwise axially symmetric system by the four orthogonally arranged baffles. p is therefore definitely a function of baffle width, but probably is influenced by more factors. For this setup, it kept in the interval $(2; 3)$. The offset of the ring centre is also computed, allowing to quantify eccentricities in the tank (e.g. off-centre mixer). A relatively close match was found between numerical and experimental approach. Introduction of p-norm might serve to deepen the theoretical understanding of similar mixing cases. On enclosed image, new MATLAB image analysis tool is demonstrated on results of an M-Star simulation. This research is financially supported from SGS23/160/OHK2/3T/12.



Glatt Ingenieurtechnik GmbH – From your product idea to industrial production

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The contributions reflect the technological expertise of Glatt Ingenieurtechnik GmbH. Potential applications will be illustrated on a poster using selected examples.

Technology for environmental protection

INNOVATIVE REMOVAL OF HALOGENATED ORGANIC ACIDS FROM POLLUTED WATER IN A SPIRIT OF CIRCULAR ECONOMY

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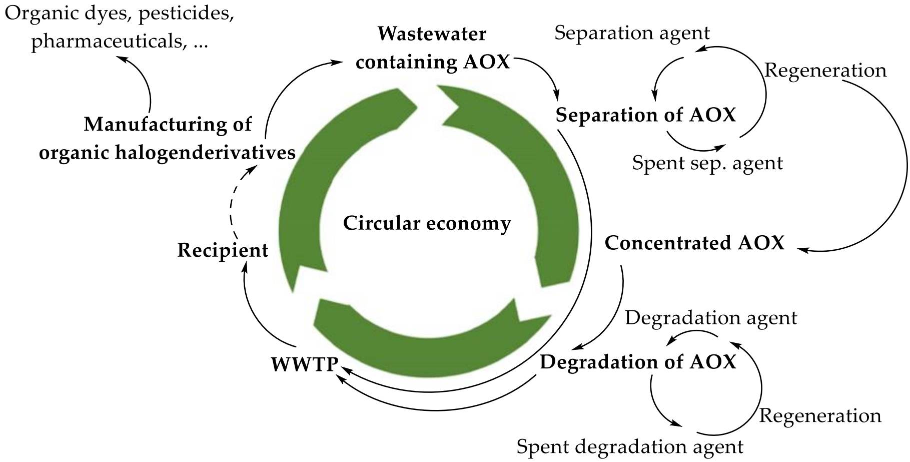
The development of industry is associated with increasing of the presence of problematic pollutants in natural water as well as wastewater. Such pollutants include, for example, halogenated organic derivatives (also known as Adsorbable Organically Bound Halogens - AOX), which are widely applied as dyes and pigments, drugs, pesticides, etc. These compounds are persistent, bio-accumulative, and generally show a low degree of biodegradability. Technological processes devoted to the limitation of AOX emissions into the environment focus on the possibilities of economic and ecological remove of these substances from contaminated waste aqueous streams. Among many technologies, adsorption on active carbon as essential separation process is commonly applied. However, alternative carbonaceous adsorbents such as biochar can be also utilized. After saturation of adsorbent, depleted active carbon or biochar has to be combusted in hazardous waste incinerators or recovered *via* pyrolysis. Thus, the thermal desorption can generate the regenerated adsorbent, but also aqueous solution of concentrated contaminants which can be eliminated using incineration or chemical degradation. This contribution presents innovative possibilities of the separation of AOX compounds using alternative sorbents and the subsequent reductive degradation of organic halogen derivatives in the spirit of the circular economy, see figure bellow.



***Acknowledgements**: This work was supported by excellent technological teams from the Faculty of Chemical Technology, University of Pardubice, No. VA390013.*

Recycling of spent dye baths used for cotton dyeing with reactive dyes

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In textile production is water used for removing impurities, dyeing process, applying finishing agents or for steam production and as a result, textile production is responsible for up to 20 % of global water pollution. Almost complete input volume of used water is discharged as wastewater stream. This wastewater usually contains significant concentration of soluble organic compounds (represented as a high value of COD and BOD), a higher total amount of dissolved inorganic salts, high pH value and it is usually highly colored. Due to these mentioned reasons the effective wastewater treatment and recycling can play a significant role in reducing discharge of pollution and providing reusable process water.

For a required migration of the dye to the fibre, it is necessary to use a sodium chloride solution. Almost total amount of added sodium chloride remains in the wastewater, therefore the ideal solution is to use this already salty water for further dyeing. To maintain quality, it is necessary to decolorize this wastewater and remove other unwanted substances. The ionic liquid Aliquat 336 is used for this purpose, which is suitable due to its physical properties. Decolorization of wastewater is carried out by precipitation using an ionic liquid and activated carbon with previous pH adjustment using a flocculant. The resulting precipitate is separated by sedimentation and filtration. Decolorized water with a certain amount of sodium chloride is obtained in this way. After addition of appropriate quantity of NaCl to the required salinity, the decolorized brine is reusable for subsequent dyeing.

Recycling of wastewater after dyeing cellulose fibres using an ionic liquid has proven to be a very convenient and relatively fast method. From an economic point of view, at this moment it is necessary to pay attention to the ratio between the amount of ionic liquid, quantity of added coagulant and quantity of applied activated carbon.

SPREADING, FORMATION AND CAPTURE OF AEROSOL PARTICLES: THE CASE OF COVID-19

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From 2020 up to 2022 the Covid-19 pandemics was a major disruptor of daily activities on the level of individuals and entire society. The statistics for Covid-19 pandemic outcomes in Czech Republic are not favorable when compared to countries emphasizing somewhat different approaches in personal protection.

In this contribution, basic physical mechanisms of aerosol particles spreading, formation and capture in fibrous filters (respirators) and in human airways (upper, middle and alveolar) is briefly explained in the framework of chemical engineering, nanotechnology, physical chemistry and computer-aided analysis.

As a conclusion, the explanation why the national 3R strategy for Covid-19 protection had a limited effectiveness is discussed based on first principles. The subjects of the analysis are individuals and common scenarios from everyday life, such as outdoor activities, staying in rooms and public transport. Material presented in this contribution was taught to students since April 2020.

GUANIDINE POLYMERS AS NITRIFICATION INHIBITORS FOR GRANULAR NITROGEN FERTILIZERS

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One of the most important elements in plant nutrition is nitrogen (N). Its content in the soil can change in a short time, which can significantly affect the harvest of farming products. Losses of nitrogen through leaching or gaseous emissions reduce the efficiency of fertilization. The N content depends on several factors, such as type of soil, climatic conditions or the sort of used nitrogen fertilizer. One of the alternatives to reduce and limit N losses is using nitrification inhibitors, which slow down or delay the oxidation of ammonia N (NH_4^+) to nitrate N (NO_3^-) [1].

The application of guanidine polymers as inhibitors of the nitrification process was not known until now. These polymers are used exclusively as biocides[2]. In the laboratories of VUCHT a.s. the properties of guanidine polymers as nitrification inhibitors of nitrogen fertilizers were studied and tested. Polymers of guanidine hydrochloride with diamine compounds were prepared, which were applied in the form of an aqueous solution on the surface of granules of nitrogenous fertilizer, or added directly to the slurry of the fertilizer before the formation of granules. A copolymer of guanidine hydrochloride polymer with 1,2 diaminopropane and ε-caprolactone as a nitrification inhibitor was also prepared and applied to granular nitrogen fertilizers[3,4].

The nitrification inhibitory effects of granular fertilizers with the addition of guanidine polymers or copolymers were determined in soil pot tests as well as in small-plot field experiments on the agricultural crops such winter wheat, winter rapeseed and seed corn.

By using the mentioned nitrification inhibitors, a significant reduction of nitrogen losses in granular nitrogen fertilizers has been achieved.

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MANAŽMENT BIOKALU NA MCHBČOV SLOVNAFT A.S.

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SLOVNAFT, a.s., Bratislava, Slovenská republika

Úvod

Mechanicko-chemicko-biologická čistareň odpadových vôd v rafinérko-petrochemickom závode SLOVNAFT, a.s. v Bratislave je v prevádzke od roku 1984. V ostatných rokoch sme sa zamerali na zlepšovanie riadenia procesu. Predchádzajúce realizácie technických opatrení, medzi ktoré patrí komplexná rekonštrukcia spaľovne kalov a rekonštrukcia aeračného systému na biologickom stupni umožnili aj zlepšovanie riadenia procesov.

V predchádzajúcom kroku sme sa venovali optimalizácii riadenia chemikého stupňa, tu popíšeme zlepšovanie riadenia biologického stupňa čistenia odpadových vôd.

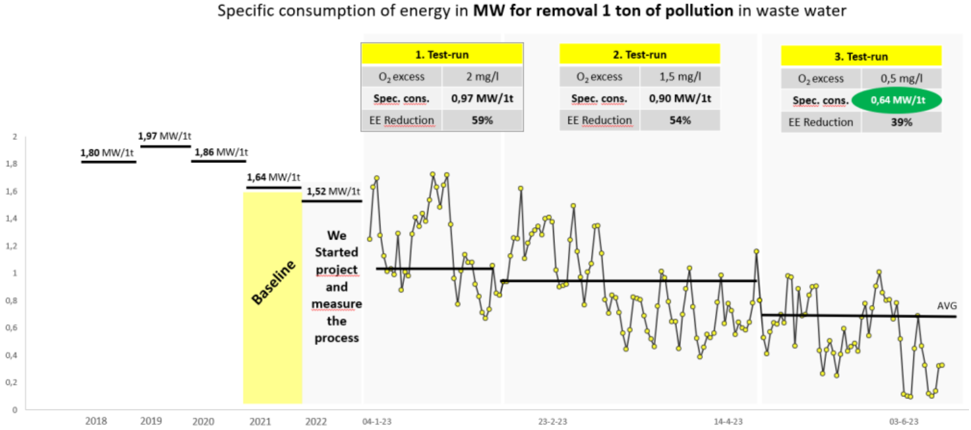
Metodika

Projekt procesného zlepšovania bol riadený metódami six sigma, s využitím techník a nástrojov štatistického spracovania údajov, riadenie zmien a overovanie prevádzkovými pokusmi.

Počiatočnou fázou bola identifikácia a overenie meracieho systému. Následne boli analyzované a v troch krokoch riadené zmeny procesných parametrov.

Prvý prevádzkový pokus bol zameraný na stabilizáciu režimu a zníženie variability procesu. Cieľom druhého testu bolo nastavenie režimu na minimálny obsah rozpusteného kyslíka v systéme pri konvenčnom režime. V treťom kroku sme overovali možnosť využitia inovatívnej metódy simultánnej nitrifikácie a denitrifikácie. V každom režime sme vyhodnocovali kvalitu, stabilitu technologického procesu a energetickú náročnosť

Výsledky



Závěr

Optimalizáciou priadenia procesu bol úspešne stabilizovaný technologický režim, pri dodržaní kvality vyčistených vôd bolo dosiahnuté zníženie energetickej náročnosti.

METHYLMERCURY EFFECTS AND ACCUMULATION IN TWO EXTREMOPHILE MICROALGAE STRAINS *COCCOMYXA ONUBENSIS* AND *DUNALIELLA SALINA* LOCAL TO ANDALUSIA (SPAIN)

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The primary entry point for highly toxic organic forms of mercury, such as methyl-mercury (MeHg) into aquatic food webs is through phytoplankton, predominantly composed by various microalgal species. Understanding the processes of MeHg intake by microalgae, the effects on population size, cell toxicity, bioaccumulation and eventual biotransformation is of greatest importance for human health, since through process of biomagnification this Hg eventually ends up in aquatic wildlife, fish, seafood and eventually human diet. This study was conducted on two extremophile microalgae strains local to southern Spain *Coccomyxa onnubense* (acidophile freshwater alga) and *Dunaliella salina* (halophile seawater alga). The exposure experiments were conducted in laboratory scale. The effects of three different concentrations of MeHg were tested during 72 h cultivation. The results are supported by photos from transmission electron microscopy (TEM) and the determination of superoxide dismutase (SOD) enzyme activity.

CHARACTERIZATION OF STRUCTURALLY DIFFERENT BORON-DOPED DIAMOND ELECTRODES

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The efficiency of boron-doped diamond electrodes (BDDE) in wastewater treatment is influenced by boron content, sp^3 carbon content, total surface area, surface morphology, etc. In addition to the rate of pollutant removal, surface characteristics can also affect the rate of formation and composition of degradation by-products. Electrode characterization can be approached by both direct surface analysis and qualitative and quantitative analysis of the reactants formed.

Microscopic techniques such as scanning electron microscopy (SEM) or digital holographic microscopy (DHM) are used to analyse the surface of BDDE. Raman or infrared spectroscopy is also frequently encountered, as well as electrochemical methods such as cyclic voltammetry (CV).

Quenching is commonly used to determine the amount and type of reagents formed on the surface of BDDE, including oxidative ones, but also electron paramagnetic resonance or methods monitoring the change in absorbance in the UV-VIS spectrum or the formation of fluorescence radiation after the reaction of a reagent with a specific organic substance. Therefore, a combination of methods describing both the electrode surface and the formation of oxidizing agents was used to characterize the newly developed electrodes.

This work was supported by project VA390013.

TREATMENT OF PHENOLIC INDUSTRIAL WASTE WATER BY CATALYTIC WET AIR OXIDATION USING A CUMNFE MIXED OXIDE CATALYST IN A CONTINUOUS FLOW REACTOR.

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Hydrotalcite-like materials (LDHs) are recognised as excellent materials for catalytic use. These materials are used in a wide range of applications, including the catalytic wet air oxidation (CWAO) process for treating wastewater. For the evaluation of CWAO waste water treatment consisting of phenol, our research tested the double layer hydrotalcite (LDH) CuMnFe catalyst for its potential application on an industrial scale. The CuMnFe catalyst was prepared by the co-precipitation method with a molar ratio of 4:1:1. Its chemical composition (ICP-OES) and textural properties were investigated by XRD and N2-physisorption before and after the tests. Two evaluation tests were carried out in a quarter scale continuous flow unit using a 1200 ppm concentration of phenol reference waste water and a diluted real industrial waste water. The concentration of phenol in the treated wastewater was analysed by HPLC every 4 hours. The concentration of metals from the catalyst was also evaluated by ICP-OES. Our tests have shown that the use of CuMnFe as a catalyst leads to a significant decrease in the concentration of phenol in the final product, especially with real waste water. Furthermore, this decrease was maintained throughout the test for 96 hours. For the sake of industrial sustainability, the operating conditions in this paper are also suggested.

EXPLORING SUSTAINABLE FUEL SOLUTIONS AND FUEL QUALITY MEASUREMENT OPTIONS

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From the point of view of environmental quality, the pressure to reduce the pollution caused by car traffic is increasing. Furthermore, due to dwindling oil reserves and the closure of oil refineries, the EU has also announced an exemption from the ban on the sale of new gasoline and diesel vehicles until 2035, which will allow internal combustion engine vehicles to run exclusively on synthetic fuels – eFuels. It appears that electric cars are not a complete alternative either, as the European Commission has found that the balance of pure electric cars (referred to as BEVs) must cover the entire life cycle of the car, including battery production and operating losses. It is also worth noting that in most European countries, coal and gas dominate electricity generation. Synthetic fuels are another option to consider. Some car manufacturers are already beginning to address this situation, such as Porsche, which has built a plant in Chile to produce synthetic fuels from water, wind, and CO_2. Fuel quality assessments include a number of methods and techniques to ensure optimal performance and environmental sustainability. One of the prevalent methods involves measuring key parameters such as octane, cetane number, and viscosity, providing insight into combustion efficiency and engine compatibility. In addition, chemical analysis techniques, including chromatography and spectroscopy, allow the identification and quantification of fuel components, which aids in the detection of contaminants. In addition, various biofuels are being added to fuels, increasing sustainability efforts. Direct monitoring of the quality of fuels in vehicles appears to be a promising approach to pollution control, facilitating early interventions to maintain quality. Furthermore, this paper presents the possibilities to measure the quality of fuels by changing the electrical properties of fuels in internal combustion engines and offers an innovative view of quality assessment methodologies.

Decarbonisation

DecarbonisationSLOVAK HYDROGEN ECONOMY – CASE STUDY OF ALTERNATIVE FUELS

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The European Union set an ambitious goal in terms of decarbonization. It is the reduction of emissions by almost 12% by 2030 compared to 2020. Today, the transport sector produces a quarter of total greenhouse gas emissions. A suitable solution offers the utilization of hydrogen, which is currently considered as the main driving force of decarbonization. This work focused on three possible alternative fuels: methanol, methane, and sustainable aviation fuel, which use hydrogen as an energy carrier. The study consists of six hydrogen production alternatives that are compared. Three of them employ are electrolysis, and the other three utilize biogas reforming as a more environmentally friendly replacement for fossil natural gas. Multi-criteria decision analysis is used as an evaluation tool with three comparison criteria: economics, environmental aspect, and maturity of hydrogen production technology. The analysis represents a feasibility study of the Slovak National Hydrogen Strategy, aiming to use 5 kt of hydrogen per year for the production of alternative fuels by 2030. Slovakia represents a typical example of a central and eastern European country with a lack of favourable natural conditions for replacing fossil energy sources with renewables. The sensitivity analysis in this work aims to identify an ideal scenario in which countries like Slovakia could compete with those that have more favourable conditions.

Proton exchange membrane electrolysis and steam biogas reforming prove to be the most advantageous hydrogen production technologies according to the selected criteria. Sustainable aviation fuel production is ranked highest among alternative fuels based on economic factor. Sensitivity analysis indicates that at least an 80 % reduction of electricity price is required to ensure the competitiveness of Slovakia in the alternative fuels market. A suitable path involves reducing the cost of electricity, necessitating the technical development of various renewable energy sources.

This work was supported by the call for doctoral students and young researchers of Slovak University of Technology in Bratislava to start a research career (Grant 23-04-11-A). Support by the Slovak Research and Development Agency under contract nos. APVV-18-0134 and APVV-19-0170 is gratefully acknowledged.

Optimalizace provozních parametrů separace CO_2 ze spalin na základě pilotních testů

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Úvod

Membránová separace CO_2 umožňuje pomocí technologie s malými rozměry recyklovat CO_2. To dovoluje zavádět cirkulaci CO_2 i v místech, kde to kvůli jeho nedostatečnému množství nebylo možné. Problematika separace CO_2 je velmi citlivá na provozní náklady, zejména na spotřebu a cenu elektrické energie. Navíc je nutné řešit otázku emisních povolenek a tzv. valorizace CO_2.

Metodika

Pilotní jednotka využívá k separaci CO_2 ze spalin membránový modul obsahující membránu s vysokou permeancí CO_2 a selektivitou CO_2/N_2. Díky tomu jde rozdělit směs CO_2 a N_2 na dva proudy, jeden obsahující hlavně CO_2 a druhý N_2. Hnací silou je rozdíl parciálních tlaků složek na opačných stranách membrány. Optimalizací provozních parametrů, jako je výkon dmychadla (nebo kompresoru), vývěvy a chlazení lze dosáhnout nízkých nákladů na separaci CO_2. Mezi jeden z hlavních konceptů se řadí i možnost provozovat technologii v režimu s nízkou koncentrací CO_2 na výstupu (kolem 50 %), který je velmi ekonomicky příznivý, nebo v režimu s vysoce koncentrovaným CO_2 (>95 %), který umožní využití CO_2 v aplikacích citlivých na jeho čistotu. Provoz s nízkou koncentrací CO_2 na výstupu byl pilotně realizován, vyhodnocen a optimalizován.

Výsledky

Pilotním testováním byly potvrzeny separační vlastnosti membránového modulu udávané výrobcem, i když byla zjištěna nižší selektivita CO_2/N_2 i CO_2/O_2. Také byl kvantifikován vliv teploty separace na výkon modulu. Zároveň byla vypracována analýza spotřeby elektrické energie a byly identifikovány provozní podmínky, při kterých dochází k maximalizaci výtěžku CO_2. Na základě testů byly nalezeny optimální podmínky i pro odlišné konfigurace technologie. Také byl popsán vliv koncentrace CO_2 ve vstupních spalinách, který zásadně ovlivňuje celkovou ekonomiku membránové separace CO_2.

Závěr

Pilotní provoz jednotky separace CO_2 ukázal na možnosti jejího využití v konkrétních aplikacích. Technologie membránové separace poskytuje dostatečně kvalitní proud CO_2 pro jeho spotřebu nebo další zpracování. Technologie umožňuje využití v místech, kde se spotřeba CO_2 pohybuje v desítkách až stovkách kilogramů CO_2 za hodinu.

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A NEW MEMBRANE FOR MIX GAS AND FLUE GAS SEPARATION

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One of main sources of industrial emissions is the combustion technology. In addition to solid waste, a number of compounds produced by the combustion leave the system in the gaseous state. At present, there are various methods for the purification of waste gases that allow flue gases released to the atmosphere to fully comply with emission standards. However, these technologies are now often reaching the maximum limits for their separation capabilities, and it is clear that with the more stringent emission limits imposed by the European Commission effective from 2021, they will not be able to meet them. The aim of this work is to test our new patented method of water condensing membrane for flue gas purification [1,2]. Moreover, our objective is also to compare our unique separation method with polymeric membranes being nowadays developed primarily for carbon capture (CC). Nevertheless, these membranes and whole CC technology have also solve the problem of the other pollutants like SO2, NOx and HX. We would like to find out whether the new separation method could be as efficient as the current polymeric membranes represented by the results of several academic investigations and pilot tests performed by membrane producers. It seems that it would be very advantageous and reasonable to develop the process combining efficient SO2, NOx, HX removal and water recovery but not necessarily with CO2 removal as CC will be possible only on sites where it could be further processed. Thus, there could be also a demand for the efficient technology without CC to be combined with current flue gas purification systems especially on smaller scales.

A unique lab-scale apparatus testing the purification of flue gas has been built. Using tested flat sheet membrane Toray, the purification of feed gas to levels required by the legislative of the European Commission since 2021, has been achieved. Various separation conditions (pressure above and below the membrane, temperature of separation, flux of feed and sweeping gas) were tested and optimal parameters were found. Our results proved high separation potential of "water condensing membrane" for separation of SO2, and CO2 from flue gas.

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DEVELOPMENT OF A DIGITAL TWIN OF A PHENOLIC RESIN PAPER IMPREGNATION PLANT DRYER

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Drying is one of the most widespread and energy intensive processes in industry. Therefore, small improvement in energy efficiency of the drying processes in general may lead to significant energy and GHG emissions savings. This work considers gas fired continuously operated flotation dryers, which are typically used in phenolic resin paper impregnation plants for manufacturing laminated panels. Inside the dryer the fabric is floating in the stream of hot air through several zones. The process is conventionally operated with excessive air to keep solvent concentrations in the exhaust gas such as methanol below their lower explosive limits. Because of the complexity of the drying process, it is not possible to directly determine the optimal operation parameters for minimum fuel consumption. This contribution presents results from the implementation of a digital twin for the production process, which links a thermodynamic model of the drying process with real-time process data. The model predicts the change in paper temperature and solvent content throughout the dryer and provides the evaporated amount of solvent in each drying zone. Linking input and output streams of the dryer and closing corresponding mass and energy balances, the developed numerical model can be iteratively fitted to available operational data by solution of a nonlinear regression problem adjusting basic parameters for heat transfer and drying curve. The successful application for the identification of optimal operation parameters for decreased energy consumption while considering the lower explosive limit of methanol is demonstrated.

MODELING AND ANALYSIS OF INDUSTRIAL STEAM NETWORK OPERATION CHANGE WITH NEW STEAM SOURCE COMMISSIONING

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Steam networks in industrial parks and enterprises usually developed over decades to their current layout, closely following the development of production. Significant changes in steam balance in such networks inevitably challenges the stability of their operation and in the quality of steam delivered to end users. Mathematical modeling can be used to provide answers to the arising queries regarding future operation of steam networks and possible modification in their layout to cope with the expected changes in steam mass flows and flow directions. This study showcases an industrial steam network which is expected to undergo a major operation change due a new low-emission steam source (60 t/h steam export capacity) commissioning. Steam export is envisioned on both middle-pressure (1 MPa) and low-pressure (0.4 MPa) level, with a notable flexibility in individual steam mass flows. A combined thermo-hydrodynamic model is applied to predict maximal export which the current steam network can accommodate in various operation states. Results indicate that all steam from new steam source can be exported to the industry in winter, achieving a proportional decrease in steam production in the existing central heat and power plant, followed by fuel saving and greenhouse gases (GHG) emissions decrease. Summer operation of the steam network in future conditions allows for a limited 1 MPa steam export (up to 30 to 35 t/h) only, while that on 0.4 MPa level will not be possible for most of the time. The remaining steam will most probably have to be used for condensing power production. Overall, around 75 % of annual steam production in the new steam source could be exported to steam network, leading to fuel saving and to a cut in GHG emissions, constituting a favorable basis for an economic operation of the new steam source.

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LESSONS FROM THE PAST: APPLICATION OF A CENTURY-OLD METHOD FOR PIPELINE NETWORKS MODELING IN INDUSTRIAL PRACTICE

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Steam turbines have served as mechanical drivers of choice in heavy industry for decades, mostly in places where abundant heat could provide energy for steam generation. These drivers have been incorporated into complex and usually multi-level steam networks which span across whole industrial plants. However, the global environmental trends, rising fuel prices, and the ever-increasing carbon tax are making the economics of steam drives operation questionable and are shifting the industry towards electrification. The switch from steam power to electro power needs to be done with caution, though, as such actions affect the steam pipeline network and the steam production facilities substantially. To assess the effects of replacing a series of installed steam turbines for high-speed electromotors, a complex study of all levels of the steam network needs to be done and any potential bottlenecks need to be addressed. The current trend in digitization pushes engineers into the world of simulations engineering, although a software capable of such calculations is often out of reach for domestic industry. Furthermore, even the most sophisticated simulation software tends to fail when trying to simulate such highly interconnected and nonlinear systems as plant-wide steam networks. Hardy Cross came up with a solution to the issue of pipeline networks modeling in the mid-1930s. Decades later, his method was deemed obsolete due to the development of computer solving methods and modern algorithms. However, almost a century later, this method was once again proven useful in a case where no simulation software or modern algorithms were applicable. This contribution presents the main results of an extensive industrial study of the impact of steam-drives replacement on the plant steam management and highlights the relevance of traditional engineering methods in modern applications.

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PRODUCTION OF HUMIC ACID FOR POTENTIAL REDUCTION OF HUMAN CO_2 EMISSIONS

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The organic matter fraction in the geological carbon pool contains an estimated 10^{16} tons of carbon, exceeding the total organic content of current living matter by a factor of 10 000. Soil contains by far more carbon than the atmosphere (currently 870×10^9 t) [1].

Soil organic matter (humic substances) is in major parts a long lasting, accumulated product of the degradation of land plants, and a change of its content in the range on larger soil areas has the potential to cure the climate crisis completely.

The humin/humic acid fraction of organic matter (above mentioned immobilized soil carbon, humic substances) in the upper layers of farmed soil contains an overall of 1500×10^9 t of carbon. For a comparison, total quantity of carbon in the atmosphere is 800×10^9 t [1].

The notation “humic acid” (HA) comes from the early chemical experience that strong bases dissolve significant parts of peat while re-acidification results in precipitation. HA is a complex polymer compound that contains acidic carboxyl and phenolate groups.

The formation of humic substances under natural conditions requires many years and involves biotic and abiotic reactions. However, HA is synthetically available.

Hydrothermal technology can rapidly convert biowaste into high-value products within hours or even minutes by creating a high temperature and high-pressure environment.

HTH usually achieves excellent carbon yields and metabolization is avoided, i.e., the majority of the carbon bound in biomass ends up in the humified product.

As synthetic HA is essentially carbon negative (it binds carbon while its formation has avoided metabolization and CO_2 generation) and it is made essentially only from side products or waste streams, application of synthetic HA as a replacements of fossil products or on larger scale in agriculture can contribute to find a way to a CO_2-neutral society.

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DEFOSSILISATION AND DECARBONISATION. THE ENERGY FRAME OF THE FUTURE OF CHEMICAL INDUSTRY VIEWED BY PHYSICAL CHEMISTRY

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Fulfilling of decarbonisation and defossilisation targets of EU and Czech Republic requires dramatic transformation not only of electricity production, but of the Czech and Central European energy industry. Approximately 400-440 TWh produced in the Czech Republic using fossil fuels will have to be replaced by low carbon emitting or/and renewably energy sources, this means that energy production from these sources have to be increased more than six-times in next twenty five years. Possibilities, risks and specific features both of autarkic and global solutions of Czech energy transformation and their impact to the Czech chemical industry will be discussed in this paper.

Výsledky pilotních testů membránové separace CO_2 ze spalin plynového kotle

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Úvod

Postupné zvyšování CO_2 v atmosféře předkládá zásadní otázku jak tento trend zastavit, aby nedošlo k negativním dopadům na životní prostředí. Proto se hledají cesty jak snížit emise CO_2 ze spalovacích procesů. K odstranění CO_2 ze spalin je možné využít procesu absorpce, adsorpce, membránová separace, případně kryogenní destilace.

Metodika

Pro izolaci CO_2 ze spalin jsme se již tradičně rozhodli použít metodu membránové separace, která využívá rozdílnou permeanci plynných složek kouřového plynu CO_2, N_2 a zbytkového O_2 průchodem přes membránu. Hnací silou je gradient tlaku na membráně, který je vytvořen na vstupní straně (Feed) dmychadlem a za membránou (Permeát) umístěním vývěvy. Tlakový gradient je velmi nízký, kolem 1,2 baru a proto jsou na membránu kladeny vysoké požadavky na její permeabilitu a selektivitu. Zařízení je umístěné v 20“ kontejneru a technologie separace je doplněna dvostupňovým chlazením kouřových plynů, odloučením a odvodem kondenzátu s jeho neutralizací, analyzátorem jednotlivých složek plynných proudů – Feed/Permeát/Retentát a řízením technologie s dálkovou správou. Jednotka byla připojena na spaliny za plynovým kotlem, které po projití ekonomizérem kotle měly teplotu 60°C. V tomto místě byla na spalinovod napojena pilotní jednotka Membrain. Spaliny byly svedeny izolovaným potrubím do technologie separace CO_2. V průběhu testů byly měněny parametry: průtok Feedu a jeho tlak, teplota separace a podtlak na straně permeátu.

Výsledky

Výsledky testů potvrdily předpokládanou permeanci membrány dle dodavatele modulu, selektivita je nižší, než se očekávalo. Nejvyšší selektivity se dosáhlo při nízkých teplotách plynu na modul v rozmezí 10–15°C, v této oblasti je ale nejnižší permeance modulu, takže není vhodné se v nízkém teplotním rozmezí plynu pohybovat. Pro průmyslové využití byla stanovena spotřeba el. energie v závislosti na účinnosti odloučení CO_2 pro jednotlivé provozní stavy.

Závěr

Při nízkém obsahu CO_2 ve spalinách plynového kotle méně jak 6 obj.% se ukazuje, že dosáhnout nízké spotřeby el. energie na separaci CO_2 bude velmi obtížné. Pro průmyslové využití separace CO_2 ze spalin se předpokládá max. spotřeba el. energie 0,6 kWh/kg CO_2.

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Ukládání tepelné energie v Glauberově soli

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Ukládání různých forem energie představuje jednu z mnoha zásadních výzev dnešního světa. Dekahydrát síranu sodného, známý také pod triviálním názvem Glauberova sůl, má schopnost uchovávat teplo, a to pomocí fázové změny. Při tomto jevu dochází k dehydrataci soli. Po zahřátí nad bod tání (32 °C) se Glauberova sůl dehydratuje a krystaly soli se rozpustí, pokud je naopak ochlazována, dojde k opětovné hydrataci a tvorbě krystalů, během níž dochází k uvolnění hydratačního tepla. Tento děj je mnohonásobně opakovatelný, navíc probíhá i za relativně malých teplotních rozdílů. Glauberova sůl disponuje velkou měrnou tepelnou kapacitou 2,7 kJ kg^{-1} K^{-1}, má ale i negativní vlastnosti. Především dochází k podchlazování, což prakticky znamená, že sůl ztrácí schopnost opětovné hydratace kvůli nízké nukleaci. To lze odstranit přidáním aditiv, jako je borax nebo aktivní uhlí, jež navíc zvyšuje tepelnou vodivost soli, ale také například mechanickým mícháním, které zabraňuje tzv. stratifikaci (oddělování jednotlivých fází).

Poster přináší poznatky z prvotních experimentů, které byly provedeny s čistou Glauberovou solí a s Glauberovou solí s příměsí aktivního uhlí. Byly měřeny teploty teplonosného média na vstupu a výstupu z akumulátoru v závislosti na čase a z těchto hodnot bylo určeno množství uloženého tepla v soli. Experimenty mají za cíl pomoci při návrhu nového typu zařízení pro ukládání tepelné energie pomocí Glauberovy soli.

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ASSESSING THE ECONOMIC FEASIBILITY OF E-FUELS: A COMPARATIVE STUDY

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In response to escalating environmental concerns and the imperative to transition towards sustainable energy sources, this contribution undertakes a comprehensive exploration of the economic viability of e-fuels, a promising alternative and substitute for fossil fuels. E-fuels, synthesized from carbon dioxide captured from industrial processes or the atmosphere, alongside hydrogen derived from renewable sources, emerge as a potentially transformative energy carrier. This study positions itself at the nexus of the evolving energy landscape, offering a nuanced comparative analysis between e-fuels, traditional fossil fuels, and battery technologies. The economic accessibility of e-fuels is examined through a cost modeling and scenario planning. By dissecting various scenarios and compare them against conventional counterparts, the study sheds light on the potential economic implications of widespread e-fuels adoption. This work delves into the dynamic interplay between cost-effectiveness, environmental sustainability, and the border evolution toward sustainable energy. This process includes a carbon capture unit, an electrolyzer to produce hydrogen gas, a plug-flow chemical reactor with a fixed-bed catalyst for the synthesis of methanol, and a distillation column. The planned capacity of the process is 400 000 liters per year. As society grapples with the urgent need for decarbonization, the findings presented here contribute to the ongoing discourse on sustainable energy solutions. This contribution not only scrutinizes the economic dimensions of e-fuels but also underscores their potential role in reshaping the trajectory of our energy future.

We acknowledge the financial support provided by Slovak Society of Chemical Engineering.

ENERGY OPTIMIZATION OF SEPARATION PROCESS FOR PRODUCTION OF ASYMETRIC ETHERS

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Organic solvents are an important part of chemical industry with ethers being among the more commonly used. One of the disadvantages of organic solvents is their environmental impact associated with both their production and regeneration. For that reason, development of solvents and processes for their production with minimal environmental impact is desired. One of such promising solvent is cyclopentyl methyl ether (CPME). This solvent could be manufactured using entirely renewable feedstock, however requiring complex separation train due to multiple side products obtained alongside CPME. Proposed separation train capable of separating these unfortunately comes with high energy requirement which increases the environmental impact of the process. This study aims at optimization of this proposed process in terms of energy consumption reduction. This is achieved through optimization of column parameters, energy integration and flowsheet changes allowing for further energy consumption reduction. By implementing several changes to process layout and operation conditions the specific heating energy required per tonne of CPME could be lowered by up to 50%. In addition, if taking into consideration other valuable products specific energy requirement decrease further.

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RECYCLING AND UPGRADING OF POLYMER MATERIALS BY SOLVENT BASED METHODS

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Plastic waste accumulation is a worldwide issue, and despite that, PET is the only polymer material that is now feasibly recycled. Polyethylene (PE) and polypropylene (PP) dominate plastic and waste production (they constitute half of the world's production of new polymers but also half of the world's plastic waste). Despite PE and PP fraction in polymer waste, we can mark PE and PP as environmentally friendly materials considering their chemical composition. Unfortunately, they are full of polymer additives containing a scale of problematic elements for recycling (nitrogen, oxygen, sulfur, chlorine, or fluorine). The purifying 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 processed polymer value. Fractionation method is also an option to separate multi-layer or composite textile materials.

Small assembled stirred pilot apparatuses were designed for polymer purification and fractionation to set various experimental conditions (pressure up to 30 bar and temperature up to 150 °C). The apparatuses are equipped with glass windows for visual control, instrumental check of polymer-solvent dissolution, or determining the cloud point. Now we are assembling a bigger apparatus to purify larger amount of polymer sample to study the mechanical properties of processed polymers.

Pilot experiments were conducted with commercial plastic waste to proof that decolorizing is possible. The experiments were successfully repeated, but plastic waste is not suitable for systematic analysis due unknown composition of used polymer additives. We have built a small laboratory extruder to prepare set of defined polymer concentration granules to calibrate the instrumental FTIR and Raman spectroscopy methods.

The textiles recycling experiments were conducted with a set of selected solvents. The decolorized samples were inspected by digital microscopy to find out the degree of decolorization. The aim is to use the low processing temperature to prevent the fiber or polymer degrading and to enable the repeated polymer recycling.

THE DEVELOPMENT OF A PLASMA TORCH FOR A HIGH-TEMPERATURE GASIFICATION REACTOR

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The global increase in energy consumption, coupled with the trend of restricting fossil fuels, has resulted in the need to discover a new, suitable, green energy source. One promising alternative fuel is hydrogen, which has a high calorific value (per unit of weight), and when utilized as fuel in a fuel cell, it produces only clear water. Hydrogen production can be achieved through various methods, with the most common being the reforming of methane or electrolysis of water. Another potential method for hydrogen production is the plasma gasification of alternative fuels. The objective of plasma gasification is to convert organic substances in fuels primarily into synthesis gas (H_2 and CO_2), while the inorganic fraction melts into an inert non-leachable slag. The integration of waste plasma gasification technology with hydrogen separation processes enables the production of what is commonly referred to as "green energy."

This research focused on the development of a new type of plasma torch for a novel gasification reactor. The first prototype of a plasma torch was constructed based on a mathematical model. The parts of the prototype had to be modified based on real operating conditions. The result of the research was a new type of functional 50 kW plasma torch, which can use N_2 or Ar as a carrier gas.

Acknowledgements

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ROLE OF THE MATERIALS USED IN A CHARGER UNIT IN THE TRIBOELECTRIC SORTING OF PLASTIC WASTE

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Triboelectric separation of plastic waste is a method that has the potential to become an important member of the plastics recycling chain for many reasons, such as the low cost of the sorting process, no use of solvents and surfactants, possible separation of black materials, etc. It uses the charging of shredded waste by contact with other objects: different plastic materials obtain a different electrostatic charge by frictional contact with a suitable counter-material. Charged pieces are then separated during free fall between electrodes in the electrostatic separator. The choice of counter-material for charging is the most challenging task in designing a triboelectric separator, as it plays a crucial role in controlling the charge of individual plastic pieces. The tribocharging of dielectrics or insulators is still poorly understood, so predicting a suitable counter-material for different waste mixtures can be challenging, so most work has to be done experimentally. Our work focuses 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. We are also investigating the effect of additives on triboelectric separation - many additives are used in the polymer industry to improve products, but these substances can cause problems during recycling. Sorting plastic waste not only by bulk material but also by specific additive content can be valuable.

THE POSSIBILITY OF HYDROTREATMENT OF PYROLYSIS OIL FROM PLASTIC WASTE

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The hydrotreatment of pyrolysis oils from waste plastics is a key process leading to a more sustainable treatment of waste plastics. These processes are an important step towards sustainable plastic material recycling and reducing negative environmental impacts. Hydrotreatment of pyrolysis oils mainly involves hydrodehalogenation and hydrogenation of double bonds (stabilisation). Hydrodehalogenation is a catalytic process that removes halogens from plastic waste, while double bond hydrogenation of pyrolysis oils aims to improve the quality and usability of the oil products from the pyrolysis of plastic materials and to enable their storage. The aim of this work is to stabilize pyrolysis oils from plastic wastes by hydrotreatment and at the same time to test the possibility of removing organically bound halogens by catalytic hydrodehalogenation. The pyrolysis oil used in this study was obtained from the pyrolysis of waste packaging materials and contained a high proportion of unsaturated hydrocarbons and 100 ppm of chlorine. This pyrolysis oil was mixed in a 1:5 ratio with heptane. Subsequently, hydrotreatment was performed on a commercially available Pd/Al_2O_3 catalyst and the efficiency of stabilisation and hydrodehalogenation at different temperatures was compared. The chlorine content was determined by XRF and the group composition was determined by GCxGC-FID. It was found that the pyrolysis oil could be efficiently stabilized and hydrodehalogenated by low-temperature hydrotreatment on Pd/Al_2O_3 catalysts at 180 °C without significant loss of catalytic activity.

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Pharmaceutical Technology

3D printing of enteric capsules using extruded hypromellose filaments

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Introduction

3D printing is predicted to play a significant role in the future of the pharmaceutical technology. Personalized drug delivery has become a new, promising and effective way in the treatment of patients. This presentation provides a contribution to the development of oral dosage forms for colon-specific drug delivery based on the hypromellose 3D printed capsules.

Experimental

This work focuses on the hot melt extrusion (HME) of hypromellose, one of the most commonly used polymers in pharmaceutical dosage forms, to prepare filament for subsequent 3D printing of dosage form. Fused deposition modeling (FDM) was utilized to produce a polysaccharide capsules using the extruded filaments. Because stability of the polymer at high temperatures during HME is of key importance, the thermal degradation of Affinisol^{TM} HPMC HME 15 LV (hypromellose specially designed for the HME) and optimum processing temperatures for HME and 3D printing was also studied.
In vitro dissolution tests with pH change (1.2 → 6.8) were performed to ivestigate the gastric fluid resistance of the printed capsules.

Results and Conclusion

Based on DSC and FTIR measurements, no significant degree of Affinisol^{TM} HPMC HME 15 LV degradation was achieved for the extrusion temperature. Printed polysaccharide (hypromellose with addition of pectin and sodium alginate) capsules are acidic resistant and show the promising application potential for colon-specific drug delivery.

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Hardening of tablets: a detective story

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Introduction

Preparation of the high API concentration tablets (80 %) is challenging for the limited amount of other additives. Nevertheless, some interactions can occur between a drug and these excipients even though used in such limited portions. On reflection, worsening of the tablet mechanical properties and the decrease in drug release can be detected.

Methods

Tablets were prepared by the compression of tableting mixture consisting of the API granules (wet granulation process) with the internal lubrication by stearic acid (intragranular) and magnesium stearate (extragranular); croscarmellose or crospovidone were added as extragranular disintegrants. Tablets were evaluated by the measurement of crushing force, disintegration time and dissolution test after preparation and during the 6 months stability study.

Results

The increase in tablet hardness following with the prolonged disintegration time and poor drug release was observed even after six weeks, particularly under 40°C/75% RH conditions of storage in a climate room. The step by step evaluation of the partially mixed substances by using MDSC showed the unexpected interaction between the drug, lubricants and disintegrant crospovidone.

Conclusions

The interaction between a drug and crospovidone was proved. This interaction, moreover, is supported by the presence of stearic acid and magnesium stearate used as lubricants. The use of croscarmellose as a disintegrant as well the exclusion of stearic acid from the composition was finally proposed.

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ROLLER COMPACTION – ADVANCES IN TECHNOLOGY TRANSFER AND SCALE-UP VIA VARIOUS METHODS AND TACTICS ASSISTED BY MATHEMATICAL MODELLING

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Abstract

Producing the same quality of intermediate products on various roller compaction machinery in dry granulation scale-up operations is essential for robust production of pharmaceutical formulations. The envelope density of the compacted ribbon, as a suitable physical property thereof, is widely accepted as criteria for transferability of dry granulation processes. Through a pilot study on a small-scale roller compactor, it is possible to prepare various batches of granulate under different process parameters to select the most preferrable batch for further development. The ribbon densities for each batch differ due to process parameters set during compaction and serve as a technology transfer parameter. The methods presented in this show how to approach various scale-up and technology transfer tactics. Several model and real formulations from the industry were compacted into ribbons, which were in turn used to evaluate the proposed method and compare it with other techniques. How to determine envelope density of roller compacted ribbons by an accurate measurement of their envelope volume by utilizing solid volume displacement of glass microspheres. It is shown that the method for envelope density measurement with solid displacement is as accurate as mercury porosimetry. The method is also resilient to different size and structure of obtained ribbon samples, including those suffering from structural failures. Product performance was also studied to generate data from the other end of the process to inspect whether it can limit design space options. Insight into how all of this data mathematical modelling is used to utilize this data will be shown in the work.

DRYING MONITORING – PAT IN TEVA

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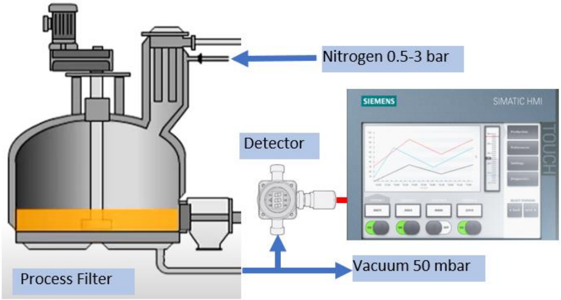
There are several options for monitoring the drying process. At TEVA, we focused on relatively inexpensive photoionization detectors (Volatile organic compound detectors) and DEW point detectors. The detectors are installed after the process filter or dryer in nitrogen stream. With their help, we can increase the drying process efficiency and understand the drying process more deeply.

The desolvation process can be monitored with this detector, as part of the polymorph control. The mobile detector can be used for troubleshooting in production. Various aspects of the detectors will be presented in the presentation and the results will be presented.



JAK CHARAKTERIZOVAT PEVNOU API VE FARMACII

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Pevnou API (Active Pharmaceutical Ingredient) charakterizujeme ve fázi preformulace vývoje léčivého přípravku. Závazná direktiva k charakterizaci neexistuje, k dispozici jsou pouze harmonizační doporučení k provedení vybraných pevnolátkových metod, obsažených v národních Pharmacopoeích (Lékopisech). Pevnolátkových analytických metod, charakterizujících práškový neboli partikulární systém, je k dispozici několik desítek. Lze je rozdělit na metody charakterizující povrch (10^{-8} – 10^{-6} m), „bulk“ (10^{-6} – 10^{-1} m) a vnitřní strukturu (10^{-10} – 10^{-8} m). Mezi parametry povrchu řadíme: povrchovou energii, reliéf (drsnost) a porozitu. Parametry „bulku“ zahrnují tvar a velikost částic, mechanické vlastnosti (pórovitost, stlačitelnost, sypnou hustotu, setřesnou hustotu atd.) a reologické vlastnosti (vnitřní a stěnové tření, kohezivitu, tokové chování, viskoelasticitu, zeta potenciál atd.). Vnitřní struktura pevné fáze je buď krystalická (uspořádaná) nebo amorfní (neuspořádaná). Parametry krystalické struktury jsou: úhly a intenzity rtg. difrakcí, Millerovy indexy rovin prokládaných atomy ve struktuře, mezirovinné vzdálenosti, rozměry elementární buňky, parametry symetrie struktury, pozice atomů v elementární buňce, příp. teplotní vibrace atomů atd. U amorfní fáze z principu krystalografické parametry neexistují a parametry povrchu a „bulku“ lze získat omezeně. Důležitým parametrem amorfního stavu je teplota skelného přechodu.

Krystalografické parametry lze získat na základě rtg. difrakčních měření, příp. z elektronové difrakce. Dostupnost krystalografických parametrů má tři úrovně:

1) Ze změřeného rtg. práškového difraktogramu získáme: úhly difrakcí, mezirovinné vzdálenosti a intenzity difrakcí
2) Indexace difrakcí: každé difrakci přiřadíme Millerovy indexy hkl a tak můžeme vypočíst rozměry elementární buňky a velmi pravděpodobně určit krystalografickou soustavu
3) Z intenzit indexovaných difrakcí (z práškových nebo lépe z monokrystalových měření) určíme prostorovou grupu symetrie, pozice atomů a příp. absolutní strukturu. Vedle rtg. difrakce lze použít i data získaná z elektronové difrakce.

První úroveň se používá např. pro potvrzení reprodukovatelnosti výrobních šarží nebo pro identifikaci API srovnáním se standardem (polymorfní chování) nebo pro zjištění stupně amortizace materiálu po mletí atd.

Druhou a třetí úroveň použijeme pro povinnou dokumentaci nebo pro korelaci struktura *vs.*vlastnosti materiálu. Důležitá je také možnost výpočtu teoretického práškového difraktogramu a jeho srovnání s experimentálním difraktogramem.

Tato práce byla podpořena GA ČR, projektem EXPRO 21-05926X

ACTIVE SUBSTANCE PRONE TO STICKING - TREATMENT IN FORMULATION FOR BETTER PROCESSABILITY

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One of the most common problems during tablet production is sticking of the material to the tabletting punches. That leads to variance in tablet weight, as well as poor tablet appearance and other quality parameters.[1] The propensity of a given active substance (API) to adhere to the equipment surfaces has to be addressed during the formulation process. To prevent API sticking, the formulation can be adjusted by altering the excipient composition, applying a lubricant coating to the API, changing the compression tooling or including additional formulation steps (such as wet granulation) in the manufacturing process.[2] Specific formulation approaches and treatments for such APIs can be protected by patents, making the generic development significantly more complicated.

In this work, we used a model API with propensity to sticking and investigated the API lubricant coating influence on the sticking phenomena. Several different lubricants were chosen for dry coating of the model API (performed by blending binary API-lubricant mixtures) and evaluation of their impact on the formulation processability was performed. To achieve that, a series of experiments with lubricant-treated API, using a compaction analyzer was performed, complemented by powder rheometry experiments of physical mixtures resembling a complete model tablet formulation.

From the used lubricants, colloidal silica presented suitable particle morphology and functional properties reducing the sticking propensity of the API, especially if further formulation steps, like wet granulation, were to be considered. Another excipient, combining calcium carbonate and hydroxyapatite (Omyanutra 300OG), having comparable functionality to colloidal silica, provided satisfying results. Moreover, more spacer-like acting excipients, magnesium aluminosilicate (Neusilin US2) and a combination of calcium carbonate and tricalcium phosphate (Omyanutra 300DC-LEG) showed some API treatment potential, which may also lead to satisfying processability with the correct formulation adjustments. Overall, two different modes of API lubricant treatment were identified as promising, potentially serving as an illustration of how to approach such sticking-prone APIs and as a base for further investigation.

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VÝROBA ANTIBIOTIK V ČESKU

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V souvislosti s diskusí o možném obnovení výroby antibiotik v naší republice bude stručně pojednáno o historii výroby antibiotik penicilinového typu v Československu a uvedeny důvody proč byla tato výroba po sametové revoluci ukončena. Dále bude popsán současný stav ve světě a diskutovány technologické možnosti či nemožnosti tuto výrobu obnovit.

KRITICKÉ ASPEKTY PŘI PŘÍPRAVĚ AKTIVNÍCH FARMACEUTICKÝCH SUBSTANCÍ

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Krystalizace je jednou z nejdůležitějších čistících a separačních metod ve farmaceutickém průmyslu. V průběhu posledních 20 let dochází ke změně v náhledu na krystalizační procesy. Se zdokonalující se technikou při charakterizaci získané pevné fáze dochází i ke zdokonalení technik, které monitorují proces krystalizace in-line. Se zdokonalující se technikou charakterizující pevnou fázi, vzrůstají ovšem i požadavky zákazníků na vlastnosti finální pevné fáze. Finální materiál by měl splňovat požadavky jak na správnou polymorfní formu, tak na velikost částic, specifický povrch a vlastnosti povrchu (měřeno např. povrchovou energií). Na základě těchto požadavků je třeba vytypovat kritické parametry, které ovlivňují finální vlastnosti materiálu. Jeden z nejzákladnějších parametrů, které je třeba kontrolovat je nukleace, což je řídící síla celé krystalizace. Existuje několik způsobů, jak parametr nukleace kontrolovat, nejpoužívanější způsob je očkování, dalším způsobem kontroly nukleace může být iniciace krystalizace ultrazvukem, případně vnesením inertního materiálu do krystalizovaného roztoku. Cílem této prezentace je ukázat, jak procesní a inženýrské parametry (teplotní rozmezí při krystalizaci, volba rozpouštědla, intenzita míchání a typ míchadla) ovlivňují vlastnosti finálního krystalického materiálu, diskutován bude i rozšířený jev objevení a zmizení nové polymorfní formy a důvody proč k této skutečnosti dochází a dále ukázat nejnovější přístrojové možnosti pro (zatím hlavně) laboratorní kontrolu krystalizace jako např. systém Blaze od společnosti Blaze Metrics, systém EasyViewer od společnosti Mettler Toledo.

IMPACT OF ULTRASOUND FOR PREPARATION OF SOLID CRYSTALLIC MATERIAL

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Crystallization of active pharmaceutical ingredients from solution is one of the most effective purification methods in the pharmaceutical industry. In order to prepare a material with desired properties (polymorphic form, particle shape, particle size distribution (PSD), specific surface area), the crystallization process must be controlled. One efficient tool to control the crystallization process is the so called sonocrystallization [1].

Firstly, ultrasound is used for inducing crystallization due to cavitation. Cavitation effectively induces nucleation and significantly improves the reproducibility of the process [2]. Further sonocrystallization advantages are shorter induction time, narrower PSD, prevent agglomeration or amorphous formation [3]. Sonication time and ultrasound amplitude tune the final particle size distribution [4]. Powder materials prepared by sonocrystallization have smoother surface, lower residual solvents content and particle shape could also be influenced.

Secondly, ultrasound is used for wet milling. Particle size is reduced directly after crystallization. Agglomerates are split and uniform distributions are achieved. Sonomilling has also positive effect on particle shape. Needle shape crystals, which are not suitable for micronization, are uniformly rounded shape and reduced after sonomilling. Sonomilling has favorable effect on homogeneity surface area and energy too compared to micronized material. Surface properties may also change the handling properties.

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ENHANCEMENT OF ENCAPSULATION AND EXTENSION OF RELEASE FOR HYDROPHILIC ANTIBIOTICS USING PLGA NANOPARTICLES VIA ION PAIRING

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Nanoparticles (NPs) composed of poly(lactic-co-glycolic acid) have demonstrated potential in the treatment of bone infections. However, hydrophilic antibiotics commonly used for local infection treatment, such as Vancomycin hydrochloride and Gentamicin sulfate, have limited interaction with PLGA. This leads to low encapsulation efficiency (EE), drug loading (DL), and a high initial burst release. To address this issue, the hydrophobic ion pairing method has been developed to achieve higher EE and sustained antibiotic release over several weeks[1,2].

This research aimed to improve EE and DL of PLGA based NPs. The HIP technique was used to investigate different anionic surfactants as HIP agents and adjusting the drug to counterion molar ratio. The Zetasizer Nano ZS was utilized to assess the size, polydispersity index, and zeta potential of the PLGA NPs. Morphology of the polymeric NPs was characterized using SEM. In addition, HPLC and UV-vis spectroscopy were employed to determine EE and DL of antibiotics in PLGA NPs and their HIP complexes. Furthermore, Particle Charge detector was used for assessing the charge of these complexes. FTIR analysis was carried out to characterize prepared complexes which revealed a notable increase in both EE and DL for highly hydrophilic antibiotics within PLGA NPs when employing the HIP method.

The study was supported by GAUK grant No. 164122/2022 and SVV 260 547. Collaboration with University of Szeged was supported by ERASMUS+

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UNEXPECTED IMPURITIES IN THE PRODUCTION OF PROSTAGLANDIN ANALOGUES TAFLUPROST

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Process impurities in the manufacture of APIs can come from multiple sources. Impurities that are associated with a chemical process - with its own reaction stage - are, from the point of view of legislation, appropriate to isolate, identify or synthesize in a targeted manner. Subsequently prove that these impurities are not present in the reaction product or in the following steps.

During the manufacture of Tafluprost (see structure **A** at **Figure 1**), which is used topically (as eye drops) to control the progression of open-angle glaucoma and to treat ocular hypertension, alone or in combination with other drugs, there is observed several impurities. These impurities were isolated and characterized. The mechanism of their formation is unknown, and our aim was to prepare these molecules by targeted synthesis. An example of such impurity for tafluprost molecule which is characterized by the presence of two fluorine atoms on the C15 carbon, is the presence of more fluorine atoms in molecule of intermediate. Fluorine atoms are introduced by reacting the corresponding carbonyl group with commercially available fluorinated agents (see structure of intermediate as **B** at **Figure 1**).

Fluorination was found not to be selective in this case and impurities were detected in which fluorine was detected in positions other than C15. The study deals with the isolation and identification of these process impurities.

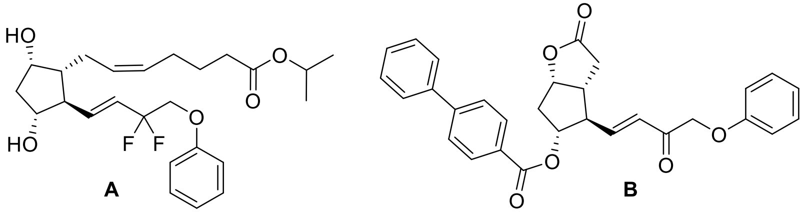

Figure 1: Tafluprost structure and intermediate for fluorination.

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PEPTIDOVÉ NOSIČE JAKO NÁSTROJ KE ZLEPŠENÍ VLASTNOSTÍ ANTIMIKROBNÍCH LÉČIV

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Rozvoj antimikrobní rezistence u řady patogenů představuje globální problém. Jednou z perspektivních možností, jak překonat tento negativní trend, je vedle vývoje zcela nových léčiv využití nových technologií na bázi drug delivery systémů (DDS).[1] Proto jsme se rozhodli zkombinovat antimikrobní léčiva s peptidovými nosiči a ověřit jejich vlastnosti.

Antimykobakteriální/antibakteriální léčiva (kyselina 4-aminosalicylová,[1] isoniazid, sulfonamidy, triklosan aj.) byla jednoduchými reakcemi modifikována tak, aby bylo možné je kovalentně navázat na peptidové DDS a současně abychom předešli vedlejším reakcím při konjugaci s nosičem. Peptidové nosiče, primárně na bázi oligotuftsinu[1-3] a jeho tandemových peptidů, byly připraveny syntézou na pevné fázi (manuální, automatizovaná) pomocí Fmoc/*t*-Bu strategie. Vzájemná konjugace nosič-léčivo byla provedene buď ještě na pevné fázi (amidová vazba), nebo po odštěpení peptidu v roztoku (oximová vazba). Konjugáty byly purifikovány a charakterizovány.

Konjugáty a samostatně i léčiva a peptidy byly hodnoceny[1] na extracelulární i intracelulární antibakteriální aktivitu, cytotoxické, cytostatické a hemolytické vlastnosti, byly stanoveny lipofilita, stabilita a buněčný uptake v modelu makrofágů.

Připravené konjugáty si zachovávaly či měly dokonce v porovnání se samotnými léčivy zvýšenou extracelulární antimikrobní aktivitu a byly nezbytné do vysokou intracelulární antimykobakteriální aktivitu. Také došlo ke zmírnění toxicity pro savčí buňky a zlepšení rozpustnosti.

Výsledky přesvědčivě prokázaly, že spojením antimikrobních léčiv s peptidovými DDS lze výhodně modulovat jejich vlastnosti, čímž dojde k efektivnějšímu využití potenciálu známých léčiv. V budoucnu budou studovány nové DDS založené na různých tandemových peptidech a jejich kombinace s dalšími typy nosičů, otevřela se i perspektiva využití pro cílení protinádorových léčiv.[2-3]

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3D PRINTED DOSAGE FORM WITH ACTIVE INGREDIENT AGAINST ALZHEIMER'S DISEASE

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Introduction

Alzheimer's disease is a neurodegenerative disorder characterised by cognitive dysfunction and dementia. According to current estimates, around 50 million people are affected by the disease.

Newly, with the aim of finding ways to increase the solubility, and thus the bioavailability, of poorly soluble drugs, which is now a highly debated topic in the field of pharmaceutical chemistry, our research group is currently focusing on the hot-melt extrusion process (HME), modifying the conditions and selecting a suitable composition. By extrusion, the crystalline form converts to an amorphous form, increasing the solubility of the substance many times over. We are also working on fused deposition modelling (FDM) 3D printing of tablets and their *in vitro* dissolution testing.

Results

A family of new compounds with a sulfonamide functional group were prepared by six-step synthesis. The ability of newly synthesized derivatives to inhibit acetylcholinesterase (AChE) from electric eel (AChE) and butyrylcholinesterase (BChE) from equine serum (BChE) was screened *in vitro* using Ellman's method and compared with that of the standard rivastigmine (RIV). Filaments containing selected active compounds were prepared by HME (see **Fig. 1**) and tablets were printed by FDM 3D printing. The dissolution test were performed in the environment simulating the human digestive tract.

Figure 1 AFFINISOL-based filament.

Conclusion

Personalized medicine offers the possibility to tailor the dose to each patient. In terms of the future, it would certainly be interesting to provide an effective and safe system for patients that could be remotely and digitally controlled by the healthcare provider.

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VARIABILITY OF PARTICLE PROPERTIES OF API AS A FACTOR DETERMINING THE OPTIMAL MIXING STRATEGY

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The direct compression process is a more economical option for tablet preparation compared to tabletting from granulate. However, in this process there are higher requirements for the preparation of a uniform mixture, as the homogeneity of the active ingredient is not fixed in the mixture, which is problematic for formulations with low active ingredient content (API). Therefore, the mixing processes tend to be very complex and usually divided into multiple steps with sieving steps included, which negatively affects the economics of the whole process.

This work included the implementation of less complex mixing processes for a formulation used for direct compression containing small amount of active ingredient. The mixing operations were performed on a small laboratory scale on Turbula® T2F 3D mixer. The homogeneity of the API in prepared mixtures was determined by analysis on high performance liquid chromatography. At the same time, the time consumption of the mixing process was evaluated based on real industrial data. All used batches of API showed different properties and therefore their variability was also evaluated. In addition to basic parameters such as particle size, an aggregation coefficient was also determined for these batches to describe the degree of representation of API aggregates in the mixture. The surface energy evaluated from the inverse gas chromatography analysis, or the cohesiveness and other parameters obtained from the shear test were also used to describe the aggregation tendencies.

It was found that all prepared mixtures were satisfactorily uniform as long as at least one sieving step was part of the mixing process. More complex processing was required for the formulation containing the API batch, which had a greater tendency to aggregate compared to the others. It was also found that not only the value of the aggregation coefficient increases with decreasing particle size, but also the cohesiveness or total value of surface energy.

SYNTHESIS OF R-(1-(6-FLUOROBENZOTHIAZOL-2-YL)-3-(METHYLTHIO) PROPYL CARBAMATES AS POTENT ALZHEIMER´S DISEASE DRUGS

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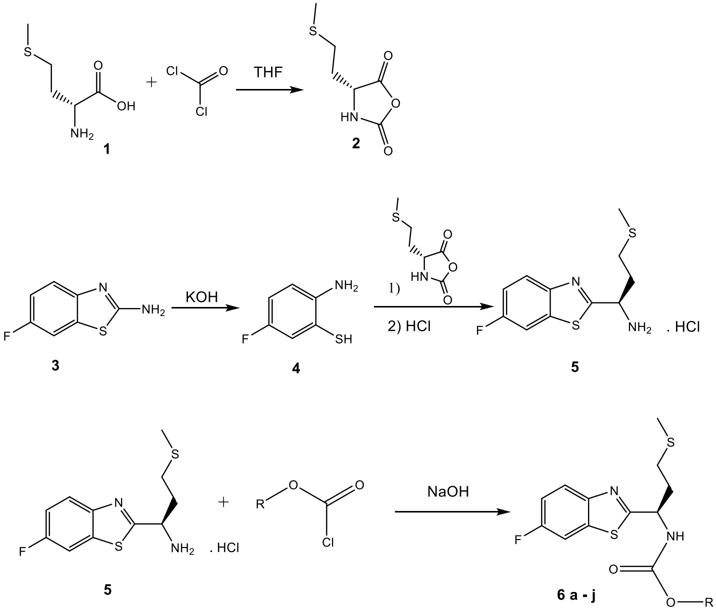
The starting compound *R*-(1-(6-fluorobenzothiazol-2-yl)-3-(methylthio)propyl) amine **5** was prepared as the corresponding hydrochloride salt. A series of novel *R*-(1-(6-fluorobenzothiazol-2-yl)-3-(methylthio)propyl carbamates **6a-j** was synthesized by condensation reaction of *R*-(1-(6-fluorobenzothiazol-2-yl)-3-(methylthio)propyl) amine with selected substituted alky und aryl chloroformates according to Scheme 1[1,2]. The structures of prepared carbamates were confirmed by ^{1}H, ^{13}C and ^{19}F NMR spectra, high resolution mass spectrometry and elemental analyses. The optical activities were confirmed by optical rotation measurements.



a) $-CH_3$
b) $-CH_2-CH_3$
c) $- CH_2CH_2CH_2CH_3$
d) $-CH_2CH_2CH_2CH_3$ (iso)
e) $-CH_2CH_2Cl$
f) $-CH_2CCl_3$
g) $-CH_2CF_3$
h) $- CH_2C_6H_5$
i) $-C_6H_5$-4-Cl
j) $-C_6H_4$-4-F

Scheme 1 Synthetic route to compound **6 a-j**.

All the prepared carbamates were tested for their inhibition of acetylcholinesterase (ACHE) and butyrylcholinesterase (BChE). The IC_{50} values were determined by the spectrophotometric Ellman's method[3]. The activities of the compounds were compared with the reference drugs Rivastigmine, Galantamine and Tacrine. The cytotoxicity of the most active compounds was investigated against human cell lines employing XTT tetrazolium salt reduction assay and xCELLigence system allowing a label-free assessment of the cells proliferation. Our results demonstrated that the inhibitory mechanism was confirmed to be pseudo-irreversible, in line with previous studies on carbamates. In conclusion, our results indicate, that these derivatives could be promising in an effective therapeutic intervention for Alzheimer's disease.

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DEPOSITION OF DRUG MICRO-SUSPENSIONS ON A POROUS CARRIER TO ENHANCE DRUG DELIVERY: THE CARRIER CAPACITY AND RELEASE EFFICIENCY

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Poorly soluble drugs, falling under BCS classes II and IV, make up a significant portion of the market. Improving their bioavailability poses a major challenge and has resulted in various strategies. One such technique is milling, which increases the specific surface area of drugs and enhances dissolution rates and overall bioavailability. The milling process follows two basic principles: the dry method and the wet method, with the latter involving liquid media to produce suspensions that offer advantages in preserving the drug's crystalline structure compared to solutions or amorphous systems.

This study centers on the preparation of interactive mixtures with a well-defined particle structure, containing an active ingredient and a porous carrier (Neusilin® US2) with specific particle characteristics. These systems provide excellent homogeneity for low-dose formulations and maximize the drug's particle surface area and its contact with the dissolution medium. However, when using a liquid medium with low wettability of the drug particles, the preparation of such systems is only successful when diluted suspensions are applied sequentially.

To achieve optimal surface coverage, we employ a hydrophilic carrier. This results in a structured surface for the prepared mixtures with higher wettability that contributes to faster drug release without requiring surfactants. This promises to even out differences in drug bioavailability when administered fasting or with food since the concentration of surfactants in the gastrointestinal tract highly depends on this aspect of administration.

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Plasty

Digitalizovaný systém třídění plastů a jeho podpora pomocí cíleného značení

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Úvod

Zrychlující se tempo klimatických změn vyvolává globální potřebu inovativního přístupu k řadě technických otázek, které dříve byly řešeny jen okrajově. Zavádění principů cirkulární ekonomiky je nezbytnou součástí řešení jedné z důležitých otázek, a to je maximálního zpětného zpracování odpadů, včetně odpadů plastových. Postupně jsou zaváděny automaticky řízené tzv. strojové třídírny plastového odpadu. Tato změna přináší na jedné straně výrazné omezení manuální práce spojené s vysokými náklady a rozsáhlou potřebou zaměstnávání nekvalifikované pracovní síly, které na trhu práce ubývá. Na druhé straně strojové třídění odpadů přináší výrazné zvýšení efektivity provozu. Strojové třídírny mohou pracovat nepřetržitě, jsou schopny vytřídit řádově vyšší objem odpadu a výrazně se zvyšuje efektivita třídění, která přináší jak vyšší čistotu vytříděných polymerních frakcí, tak výrazné snížení objemu tzv. výmětu, tedy odpadu, který není možno dále recyklovat a zatím je spalován, i když se množí aktivity zaměřené na jejich využití v jiných průmyslových odvětvích. Současný systém třídění založený na identifikaci jednotlivých druhů polymerů využívá spektrální charakteristik v oblasti VIS a NIR. Jejich kombinací je možno vytřídit převažující většinu plastů. Stávající systém není v současné době schopen vytřídit směrem k recyklaci směsné polymerní výrobky, vícevrstvé fólie nebo obaly na potraviny, ve kterých jsou kombinované různé typy polymerů. V současné době je tento typ odpadů vytříděn jako nerecyklovatelný a většinou spalován. Zvýšení účinnosti separace by mělo přinést cílené značení markery, které jsou s polymery kompatibilní, jsou na bázi organických sloučenin připravených z obnovitelných zdrojů, a vyrobitelných v EU. Tyto markery nesmí ovlivňovat vizuální prvek obalů, jejich stabilita musí odpovídat potřebám recyklačního cyklu a nesmí mít žádný vliv na mechanické vlastnosti výrobku a to ani v případě následného recyklačního procesu.

Metodika

V rámci screeningu současné situace v oblasti třídění plastů a práce s recykláty byly identifikovány tři oblasti, ve kterých je v současné době zájem o použití markerů:

1) Obaly na potraviny jsou vybaveny obtížně odnímatelnými etiketami, které jsou založeny na jiné polymerní matrici než tento obal. Potisk markeru na etiketu, který je možno provést při její výrobě v průmyslových tiskárnách, by umožnil včasné vytřídění tohoto odpadu. Následně je technologicky schůdné navrhnout oddělení obou typů polymerů od sebe a jejich vrácení do recyklačního řetězce.
2) Řada bariérových fólií nebo obalů je tvořena vrstvami různých typů polymerů. V současné době nelze tento typ odpadu využít v recyklačních technologiích, ale lze si představit jejich následné sekundární využití. V třídicím procesu je výhodné

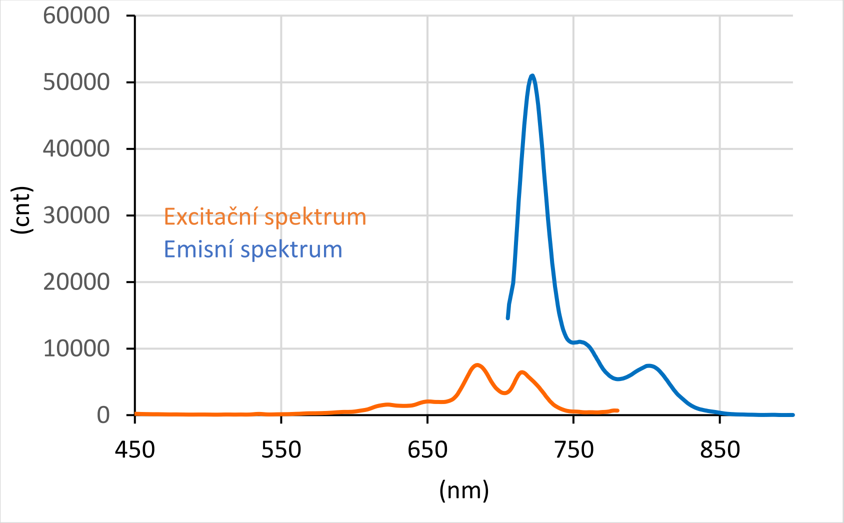
tento tytp odpadu odseparovat na začátku třídícího procesu. S ohledem na směs různých polymerních materiálů je třeba provést značení, a to nejlépe ve hmotě.

3) Zpracovatelé recyklátů mají zájem o jejich značení, což by umožňovalo kontrolu obsahu recyklátů v nových výrobcích. Zavedení markerů, které budou schopny poskytovat reprodukovatelnou fluorescenční odezvu, jejíž výše by odpovídala koncentraci recyklátů ve výrobku, by umožnilo kontrolu zda daný výrobek nebo výchozí granulát obsahuje deklarovaný obsah recyklátu.

Výsledky

Byla navržena skupina organických kolorantů na bázi ftalocyaninů a perylenů, jejichž struktura byla upravena tak, aby jejich absorpční maximum bylo posunuto na okraj viditelného spektra a absorbované záření emitovalo ve formě fluorescenčního záření v blízké infračervené oblasti 700 až 900 nm. Tak je zajištěno, že markery jsou ve výrobcích jen velmi omezeně viditelné pouhým okem, avšak snadno detekovatelné jednoduchými spektrálním metodami tak, aby byla zaručena rychlá odezva při separačním procesu. Příklad spektráln í charakteristiky testovaného markeru je na obr. 1.

Testované markery byly ověřeny po zapracování do polyolefinických substrátů nebo ve formě potisků. Současně byly markery testovány pro značení polyesterových přízí a tkanin pomocí tzv. disperzního barvení.



Obr. 1 Příklad spektrální charakteristiky markeru na bázi ftalocyaninu

Závěr

V laboratorním měřítku byly navrženy organické markery pro značení recyklátů a některých typů plastového odpadu tak, aby bylo dosaženo zefektivnění třídicího procesu. Systém je v současné době testován z hlediska dlouhodobé stabiltiy a reprodukovatelnosti tak, aby bylo možno v nejbližší době přistoupit k provoznímu testování. Systém značení recyklátů je v rámci projektových aktivit připravován ve spolupráci s průmyslovými subjekty, které zajišťují technickou podporu pro strojové třídírny plastů a současně je předmětem diskuse tak, aby vyhovoval legislativnímu rámci i s ohledem na jeho dynamické změny.

Grantová podpora
Tento projekt je spolufinancován se státní podporou Technologické agentury ČR v rámci Programu Národní centra kompetence (č. projektu TN02000051).

Polymers composites

SULPHUR VULCANIZATION OF RUBBERS

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The discovery of vulcanization of natural rubber with sulphur was a crucial step for the start of rubber industry. For mass production it was and still is desirable to improve the vulcanization process and the properties of the resulting cured rubber. Initially, the development was done by trial-and-error method. A more sophisticated approach, based on efforts to understand the chemical nature of this process, gradually gained prominence. However, vulcanization has proven to be a very complicated process and still remains a significant scientific challenge. An overview of the current state of research results in this area and the resulting potential for an approach to create tailor-made materials with a lower environmental impact will be given.

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THE INFLUENCE OF ZINC COMPOUNDS ON VULCANIZATION

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Zinc oxide is an important material in rubber industry, where it is used mainly as activator of sulphur vulcanization. It cumulates in the environment and that becomes a problem because it’s toxic for water organisms. That’s the reason why there is an effort to reduce the amount of zinc oxide. This work focused on the activation of sulphur vulcanization by zinc compounds. In addition to the commonly used zinc oxide and zinc stearate, other zinc compounds were tested with different ratios of coactivator. The vulcanization behaviour – course and kinetics was studied on the prepared mixtures, followed by the determination of the crosslinking density of the vulcanizates.

Tento článek byl vytvořen za podpory projektu NCK pro průmyslový 3D tisk, reg. č. TN02000033, který je spolufinancován se státní podporou Technologické agentury ČR v rámci programu Národní centra kompetence.

POSSIBILITIES OF 6PPD REPLACEMENT IN THE RUBBER COMPOUNDS

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6PPD (N-[1,3-dimethylbutyl]-N'-phenyl-p-phenylenediamine) is important constituent of the rubber compounds. It is distinguished by its excellent efficiency, because it acts as the antioxidant and antiozonant simultaneously. This advantage motivates its worldwide application.

However there are serious signals indicating the toxicity of this substance and mainly the quinone formed by its oxidation. The proven toxic effect on the Coho salmon gave the first alert. Following extensive research have shown adverse effects on the nerves, heart, lungs or intestines of the fishes and mammals. The abrasion of tyres is considered for the main source in the environment.

The negative effects motivated the search for the alternative antioxidant / antiozonant.

Following strategies are applied:

1. Design of structures preventing to the formation of the toxic quinones
2. Modification of rubber compounds by the reinforcement with carbon nanotubes, which enables to apply less efficient but ecologically safe antioxidants
3. Application of antioxidants of the native origin.

DUSLO is important producer of 6PPD and the issues related to the potential toxicity of this substance motivate the company to join the effort in the looking for the alternative. VUCHT, the daughter company of Duslo, has potential to design the structure replacing 6PPD and develop the technology of its production. The cooperation with the rubber compounders is necessary to achieve successful transition from the 6PPD to the less harmful alternative.

TREATISE ON DEVULCANIZATION OF WASTE RUBBER

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The ever-increasing amount of rubber waste is a global problem of today. Annual consumption of natural and synthetic rubber has exceeded 30 million tonnes. 60 to 70% of this amount is used for tyre production, the rest for manufacture of hoses, belts, gaskets, footwear, latex gloves, etc. Rubber waste therefore comes mainly from discarded tyres, the annual global increase being around 20 million tonnes. Rubber cannot be recycled easily because it is constituted of rubber chains which were crosslinked to form a spatial network during the vulcanization, becoming insoluble and infusible. Reclaiming process has been conducted for more than 150 years, consisting in scission of both crosslinks and rubber main chains, which leads to rubber degradation, however. Thus, the crucial issue of rubber recycling is to find the way how to cleave the crosslinks only, without cleaving rubber backbones; in other words, to explore the ways of devulcanization. Various methods of devulcanization have been developed but they have not reached global application yet. The paper brings on overview of the existing and perspective devulcanization methods. It also focuses the assessment methods of devulcanization efficiency.

USE OF WASTE LIGNIN FOR MODIFICATION OF CONIFEROUS WOOD TO INCREASE FIRE RESISTANCE

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In current ecological and circular economic trends, emphasis is placed on recycling and innovative use of waste materials from industrial production. Waste black liquor or waste cook acid from pulp production, rich in lignin, represents one such material offering significant potential for ecological utilization. This paper explores waste cook acid and alkaline waste black liquor for wood impregnation to enhance fire resistance and optimize its properties for further processing. We focus on analyzing the total combustion heat, where for reference spruce, a combustion heat of 19.58 MJ/kg was measured, with impregnation by waste sulfite acid estimated at 19.14 MJ/kg and by waste kraft black liquor estimated at 18.39 MJ/kg, resulting in a 6% decrease, similar trends were observed in pine wood. Other parameters monitored include the properties of the wood surface and the rate of smoke production in case of fire. Lastly, the ability of the lye to bind to the wood was observed. The aim is to demonstrate that these waste acids and liquor can be used without additional modifications, representing a benefit not only for the wood processing industry but also for ecology and the support of circular economy principles.

RECENT PROGRESS IN POLYESTER AND POLYAMIDE NANOCOMPOSITES WITH 2D FILLERS

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Industry 4.0 puts increasing demands on materials properties. Therefore, many researchers are focused on the development of materials with enhanced properties by the addition of various fillers, including 2D nanofillers with high surface area and other superior properties. This is possible due to the recent progress in synthesis of 2D materials in medium-scale quantities. This work presents the latest research on polyester and polyamide nanocomposites with 2D fillers and compares their properties with larger fillers with corresponding elemental composition (e.g. graphene to graphite).

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NANOSTRUCTURED Cu/PEN COMPOSITE: LASER-TEXTURED SURFACE AND ANTIBACTERIAL POTENCIAL

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With polymeric materials finding increasing utility across various industries, the demand for precise preparation methods and tailored properties is paramount. In this study, we engineered the surface of polyethylene naphthalate (PEN) by incorporating copper nanowires, achieved through a process involving KrF excimer laser treatment to induce coherent ripple patterns on the PEN surface, followed by copper deposition via vacuum evaporation. Surface characterisation using atomic force microscopy and scanning electron microscopy unveiled the morphology of the resulting nanostructures, while energy dispersive spectroscopy and X-ray photoelectron spectroscopy elucidated the distribution of copper within the nanowires and its gradual oxidation. The hydrophobic character was evaluated using the sessile drop method, crucial for exploring biological responses. The antibacterial efficacy of the copper nanowires against *E. coli* and *S. aureus* was demonstrated by a 24-hour incubation and drop plate test. Our findings highlight the efficacy of combining laser surface texturing and vacuum evaporation as a straightforward approach for fabricating copper/polymer nanocomposites, holding promise for bioapplications. However, it's noteworthy that significant post-deposition oxidation of the copper nanowires occurs, potentially paving the way for novel biological applications.

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SYSTEM FOR REDUCING THE ENVIRONMENTAL IMPACT OF RUBBER WASTE PROCESSING

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The project aims to create a robust recycling system for rubber waste and its digital counterpart, focusing on optimizing recyclate quality while minimizing environmental impact, including the recycling of waste textiles from End-of-Life Tires (ELT). Equipped with advanced machinery and a responsive control system, the physical line will adapt recycling processes based on sensor data. Data will be analyzed in a Cloud or On-Premise database to meet specific customer needs. The digital twin will offer versatility throughout the line's lifecycle.

TESTING OF THE DESINFECTANT ACTIVITY OF COMPOUNDS BASED ON BIODEGRADABLE OLIGOMERS

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The demand for disinfectants increased during the COVID-19 pandemic. However, their overuse and misuse has also increased. This can exacerbate the problem of antimicrobial resistance, but also have serious consequences for ecosystems and human health. An ideal disinfectant should be effective at low concentrations, be safe for human health and be effective against a wide range of micro-organisms. It should also be readily degradable, environmentally friendly, and inexpensive to produce, which lactic acid biopolymers could fulfil. Today, biopolymers are important mainly because they are renewable and non-toxic. In a normal laboratory, the bacterial effectiveness of a disinfectant can be demonstrated using the method described in the ČSN EN 13727+A2 standard.

The first step was to determine the minimum inhibitory concentration (MIC) using the dilution method in 24-well plates. The MIC was determined for four microorganisms - *Escherichia coli* (CCM 4517), *Staphylococcus aureus* (CCM 4516), *Pseudomonas aeruginosa* (CCM 7930), *Enterococcus hirae* (CCM 4533). Thirteen substituted lactyl lactates synthesised at the Department of General and Inorganic Chemistry of the University of Pardubice were thus tested. Only one of them was further tested according to the ČSN EN 13727+A2 standard.

The most promising sample was tested according to ČSN EN 13727+A2 standard in 1.5% and 2% concentration. The 2% concentration of the tested substance was not effective against Enterococcus hirae. At the same time, the sample was sent to an accredited EMPLA laboratory. There, according to the standard ČSN EN 13727+A2, the tested substance met the requirements for reduction in a 3% concentration.

The tested sample shows a bactericidal effect even in a low concentration (3%) compared to, for example, alcohol (30%) or povidone-iodine, which is typically produced in a concentration of 7.5-10%.

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NATURAL RUBBER VULCANIZATION ACTIVATED BY DIFFERENT TYPES OF ZINC OXIDE

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Natural rubber is one of the most important materials in the rubber industry. Its most important reaction is vulcanisation. To increase the speed and lower the temperature of vulcanisation, special chemical compounds called activators are used. The most commonly used activator for sulphur vulcanisation of natural rubber is zinc oxide. Zinc oxide has a very good ability to activate vulcanisation at a relatively low cost, but its main disadvantage is its toxicity to aquatic organisms. Zinc oxide is released into the environment during the production, processing and use of the products (e.g. tyres). For the cured rubbers, vulcanisation systems have been used which differ only in the different types of zinc oxide used. The influence of particle size, particle size distribution, specific surface area and particle morphology on vulcanisation and cured rubber properties was studied. Rubber vulcanisation kinetics and cross-link density of cured rubbers were investigated. Mechanical properties such as tensile strength and hardness were also evaluated.

RECYCLING OF PTFE WASTE PRODUCTS

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Nowadays, general emphasis is placed on the recycling of metallic and non-metallic materials, which is an important step towards the sustainability of natural resources and environmental protection. Recycling makes it possible to reduce costs in the production of new products and reduce the environmental burden. Poly(tetrafluoroethylene) (PTFE) is a polymer with exceptional properties, thanks to which, in combination with fillers (e.g. glass fibers, bronze powder, graphite, etc.), it finds a unique position in the industry as a material for e.g. tribological components. It is conventionally processed by pressing, sintering and then machining to final dimensions. During production, a large amount of chips is produced, which end up in the waste, as well as possible scraps or products at end of life. Recycling methods based on depolymerization or gamma ray irradiation are highly uneconomical and unfeasible for most companies. Since PTFE is very stable, the method of crushing and pulverizing into very small particles with dimensions close to PTFE raw material and their repeated use in production appears promising. To use this method, it is necessary to determine the optimal parameters of mechanical recycling, processing and verification of final properties.

In this work, several grinding processes for PTFE-based waste products for recycling were tested. The particle size of the recycled material was verified using microscopy and the purity was verified using differential scanning calorimetry. Different ratios of recycled material to the original mix have been proposed. The recycled material was mixed with the original raw material and the resulting mixtures were checked for homogeneity. In the end, a proposal for a technological procedure for the processing of mixtures, the so-called resintering, was carried out.

GRINDED WALNUT SHELLS AS RUBBER FILLER

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The pressure to use raw materials from renewable sources in rubber industry is increasing. This study is focused on the use of grinded walnut shells as a filler in natural rubber blends. Now walnut shells are an effective natural abrasive in sandblasting, polishing, and cleaning of hard materials such as metal, carbon fiber or concrete and walnut shell powder has cosmetics applications, mainly as an exfoliant.

The rubber blends were prepared with 3 different concentration of walnut shell powder. To comparison was prepared another set of blends with common filler calcium carbonate and also unfilled rubber blend. In these blends, the influence of filler on the course of vulcanization and properties of the vulcanizates has been monitored. An extrusion test was performed using a single-screw extruder.

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BIOPOLYMER-BASED FDM 3D PRINTING

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FDM 3D printing technology is gaining ground only slowly in the field of preparation of pharmaceutical forms. The use of its potential is limited by the high demands of the pharmaceutical industry. Although the selection of input raw materials is limited by this, filaments (feedstock for a 3D printer) can be made from materials already introduced in the production of dosage forms and used to print dosage forms with various dissolution properties. In addition, by combining different filament components, the properties of the products can be optimized and a specific dissolution profile can be targeted. Therefore, the product can be individually tailored to the patient's needs not only on the basis of dosage form geometry. Some components can enable or improve the processing of other raw materials the introduction of which would otherwise be accompanied by technical problems or is not completely suitable for FDM 3D printing. We, therefore, deal with the optimization of the composition of the filaments and the conditions of their preparation with the aim of designing ones from which it will be possible to print pharmaceutical forms based on an easily editable CAD model. For 3D-printed forms, we monitor the dissolution properties with regard to the pH of the environment to which these forms are exposed after administration.

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DETERMINATION OF THE ANTIMICROBIAL EFFICIENCY OF COATINGS BASED ON ACRYLATE LATEXES WITH DISPERSED NANOPARTICLES OF CONDUCTIVE POLYMERS AND SELENIUM.

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This work discusses the antimicrobial effectiveness of polyacrylate coating films containing selenium nanoparticles, conductive polymers and other nanoparticles depending on their chemical composition and concentration. First, an ecologically sound binder based on acrylate monomers was prepared using the emulsion polymerization technique, for which the basic characterization of its properties was evaluated. The stability of the colloidal system was determined. In addition, model coatings containing nanoparticles of ZnO, La_2O_3, ZnSe, SeO_2 and conductive polymers, polyaniline phosphate and polypyrrole phosphate were prepared. Model paints were applied to glass and steel panels and their physical-mechanical, chemical and corrosion resistance was tested. To determine the antimicrobial properties, loose films were created by pouring paint materials into silicone form, from which test squares were subsequently made for antimicrobial testing. The antimicrobial performance of the coating films was evaluated using the ISO 22196 method and two bacterial strains, *Staphylococcus aureus* and *Escherichia coli*, were used. The results of individual tests show that all coating films were very flexible, there was no damage or cracking, they were also relatively shiny, not too hardness and resistant to chemical agents. Coating films containing ZnSe and SeO2 nanoparticles were resistant to corrosion. From the results of the antimicrobial activity assesment , the samples with the content of ZnSe and SeO_2 nanoparticles met the parameters given by the ISO 22196 standard.

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COMPOSITE MATERIALS WITH ANTIMICROBIAL PROPERTIES BASED ON BIODEGRADABLE POLYMERS

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Biodegradable polymers have been developed as an alternative to non-biodegradable polymers and are used in a variety of applications, including food packaging, food containers, farming films, garbage bags, for filtration devices, hygiene and protective clothing. They are of great importance in the biomedical field for use in drug delivery systems, wound healing products, and surgical implant devices such as stents and others [1,2]. Their significant advantage is the ability to biodegrade into non-toxic small molecules in the presence of microorganisms and hydrolytic enzymes but also by simple chemical hydrolysis. In this work two groups of (nano)composite materials with antimicrobial properties based on biodegradable polymers will be presented. Polylactic acid and polycaprolactone were used to prepare (nano)composites with modified vermiculites, inorganic nanoparticles (Ag and ZnO) and graphene oxide. Antimicrobial properties against selected microorganisms and degradation behaviour were tested. The primary intention was to use the materials for the production of stents applicable in the digestive system, but they are considered multifunctional materials with a higher spectrum of uses [3,4,5].

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KOMPOZITY BAKTERIÁLNÍ CELULÓZY A POLYPYRROLU PRO ÚČINNÉ ODSTRANĚNÍ ŠESTIMOCNÉHO CHROMU

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Šestimocný chrom je důležitou surovinou při zpracování kovů, kůže nebo chemikálií. Jeho toxicita je však problémem nejen pro životní prostředí, ale i pro člověka. Šestimocný chrom je prokázaným původcem rakoviny plic a řady dalších zdravotních problémů. Z tohoto důvodu je použití šetimocného chromu limitováno evropskou směrnicí 2002/95/ES.

V současné době existuje poptávka po biopolymerních nebo biokompozitních materiálech, které by šlo využít pro čištění odpadních vod. Tyto materiály jsou totiž biodegradabilní, netoxické a nezávislé na ropných zdrojích. Jedním z takto využitelných materiálů je bakteriální celulóza. Její výhodou je možnost ji připravit s využitím odpadních zdrojů. Je produkována extracelulárně a mnoha bakteriálními kmeny, což z ní činí relativně snadno dostupný materiál. Jedná se o vysoce porézní materiál vhodný pro adsorpce. Pro adsorpci kovových iontů je však třeba modifikovat povrch BC.

Jedním z vhodných adsorbentů je polypyrrol. Jde o jeden z nejstudovanějších vodivých polymerů s využitelností pro čištění vod. Standartně se však vyskytuje a je připravován v práškové formě, která neumožňuje snadnou separaci z čištěné vody. Z tohoto důvodu jsou připravovány nosiče polypyrrolu ve formě aerogelů nebo kryogelů.

V této studii byly připraveny kompozity BC a polypyrrolu, které byly použity pro adsorpci šestimocného chromu. Kompozity byly následně charakterizovány z hlediska morfologických, reologických a adsorbčních vlastností. Dále bylo prokázáno, že tyto kompozity jsou vhodné pro fotokatalytickou redukci toxického šestimocného chromu na chrom trojmocný.

Tato práce byla podpořena vnitřním projektem VUT v Brně FCH-S-24-8597.

DEVELOPMENT OF BIODEGRADABLE MATERIALS BASED ON STARCH WITH NATURAL FILLERS

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Plastics nowadays are widespread in almost all spheres of human activity. Manufacturing of them is 99% based on fossil fuels. Unfortunately, that resource is known to be non-renewable. Besides that, weak point plastics based on fossil fuels have another critical disadvantage as sluggish decomposition for hundreds of years. This causes irreversible damage to the environment, because of plastic pollution all around the world. Thus, to reduce the negative influence of plastics on the environment, we have proposed the development of a material based on starch, which is biodegradable, and it is one of the most abundant polysaccharides on the planet. In this work, the structure and characteristics of starch and its modification with biodegradable fillers will be introduced. Through further processing, raw starch can 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 such (sugar beet pulp, winery wastes grape pomace (GP) and barley pulp (BP) from brewery spent grain (BSG). The optimal conditions for the modification process and the ratio of the initial components were determined. Obtained material could have promise for applications in various fields such as biomedical, packaging, agriculture etc.

Key words: thermoplastic starch, biodegradable filler, sugar beet pulp, grape pomace, barley pulp, brewery spent grain.

SYSTEMATIC ASSESMENT OF LIGNIN SOLUBILITY FOR NANOPARTICLE PREPARATION FROM VARIOUS SOURCES

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Lignin, is one of the most abundant biopolymers on Earth, primarily arises as a by-product within the pulp and paper industry. Despite its prevalence, lignin is underutilized, lacking value-added applications. Nevertheless, lignin holds significant promise for diverse applications owing to its distinctive aromatic structure and properties, including antioxidant potential and UV shielding capabilities.

Understanding lignin´s type, structure, and properties is crucial for its optimal utilization. Of particular importance is the assessment of lignin solubility, a property often evaluated through Hansen solubility parameters (HSP). Utilizing graphical methods, HSP aids in identifying suitable solvents for lignin.

This study focuses on characterizing various lignin types acquired through different extraction methods (Kraft, Organosolv, Alkali, Soda). Determination of HSP facilitates solvent selection for lignin nanoparticle synthesis. Dimethyl sulfoxide exhibited the highest solubility for isolated lignin, while a tetrahydrofuran-water mixture showed promise for nanoparticle preparation. Various nanoparticle preparation methods and the impact of lignin concentration on particle size and stability were evaluated. Nanoparticles smaller than 50 nm were synthesized, with dialysis yielding more stable particles and decreasing lignin concentration, resulting in diminished particle size.

The primary objective was to fabricate lignin nanoparticles with potent antioxidant properties, which were assessed via the ABTS radical scavenging assay. Comparative analysis revealed significant variations in antioxidant activity among lignin sources, underscoring the importance of source-specific considerations. Given the distinct physical and chemical attributes of lignin from different sources, the selection of a particular lignin type becomes imperative for specific applications.

The presented work was supported through the internal Brno University of Technology project FCH-S-24-8526.

Ekonomice of chemical industry

Vývoj odvětví chemického průmyslu (CZ-NACE 20) v České republice za období 2020-2022

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Pozice odvětví chemického průmyslu (CZ-Nace 20) je výjimečná v tom, že zasahuje svou produkcí do téměř všech oblastí ekonomiky.

Odvětví chemického průmyslu (CZ-Nace20) České republiky se v roce 2020 potýkal s významným poklesem výkonnosti, přibližně 25,3 % oproti roku 2019, v oblasti produkce spojených s přijatými omezeními, jejichž cílem bylo omezit šíření viru SARS-CoV-2. Další významný pokles odvětví zaznamenal v roce 2020, kdy odvětví vykázalo ztrátu ve výši 2,96 mil. Kč. Naopak v investicích dochází k mírnému růstu, a to přibližně o 5,98 % v roce 2020 oproti roku 2019. Naopak rok 2022 přináší obrat, kdy produkce vykazuje výrazný růst, a to přibližně o 31,9 % oproti roku 2021.

Příspěvek je zaměřen na vývoj vybraných finančních ukazatelů a vývoj zaměstnanosti chemického průmyslu ve srovnání s celkovým zpracovatelským průmyslem za období 2020-2023.

Analýza zahraničního obchodu komodit z chemického průmyslu České republiky s vybranými zeměmi za období 2019-2022

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Bilance zahraničního obchodu České republiky vykazuje v rámci sledovaného období pasivní saldo. V roce 2019 vykázala Česká republika pasivní saldo se zeměmi EU v hodnotě přibližně minus 97,1 mld. Kč, oproti roku 2022, kdy bilance dosáhla hodnoty mínus 89,8 mld. Kč. Přičemž nejvýznamnější propad bilance byl zaznamenán v roce 2020. Nejvýznamnějším a největším partnerem v rámci zahraničního obchodu s Českou republikou je Německo, dále Čína a Francie. Nepříznivý výsledek na stav zahraničního obchodu má obchod s ropou, zemním plynem a základními kovy.

Příspěvek je zaměřen na analýzu zahraničního obchodu komodit z chemického průmyslu České republiky s vybranými zeměmi za období 2019-2022. Analýza se zaměřuje na meziroční porovnání významných komodit chemického průmysl pro zahraniční obchod s Německem, Ruskem, Čínou, Ukrajinou, Tureckem a Visegrádskou čtyřkou.

IMPACTS OF CLIMATE CHANGE ON CHEMICAL ENTERPRISES

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Climate change is becoming an undeniable fact and affects every individual, the public and industrial enterprises. Rising temperatures caused by greenhouse gas emissions create a number of direct impacts on the operations of industrial enterprises and force them to respond to changing climate conditions. Deterioration of access to quality water, protection against extreme manifestations of climate change in the form of floods, extreme wind or long-term tropical temperatures, forces management to introduce mitigation and adaptation measures to climate change at the corporate level. In addition to the costs of decarbonisation of industry and the obligation to purchase emission allowances, a considerable part of the funds must therefore be spent on the direct effects of climate change. The degree of threat from climate change and the impact of adaptation measures on the economic performance of industrial enterprises was mapped by qualitative research in a selected chemical enterprise. The fundamental consequences of climate change for industrial enterprises were identified, as well as the adaptation and mitigation measures being adopted.

Projekty naplňující cíle udržitelnosti a přechod na cirkulární ekonomiku v podmínkách chemického průmyslu

PROJECTS FULFILLING THE GOALS OF SUSTAINABILITY AND THE TRANSITION TO A CIRCULAR ECONOMY IN THE CONDITIONS OF THE CHEMICAL INDUSTRY

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Abstrakt

The term sustainable project has been commonly used for a very long time. However, a project focused on sustainability, i.e. the circular economy, is something else. In practice, this connection occurs for a significantly shorter period of time. And that is the focus of this post. In it, the authors build on their previous qualitative research characterizing the impact of the bio-base / circular economy on chemical companies. This contribution summarizes the findings of the transition from a linear to a circular economy with the aim of enhancing competitiveness for chemical enterprises. It will be a guide to the concept of a corporate project system focused on the principles of "green chemistry" and the process of integration into the circular economy.

DIGITAL WELL-BEING AND THE TOOLS TO MAINTAIN IT

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Occupational health and safety is an issue that every company in the European Union has to address. In the Czech Republic, this is an area on which over 70 laws, decrees, and government regulations have been published since 2000 alone. While the original focus of OSH was mainly on the protection of physical health, over time it has also become oriented towards mental health. In 2018, ISO 45 001 came into force, which added physical and mental well-being into the OSH management system. However, digital wellbeing, i.e. the ability to use digital tools and social networks in a way that does not limit one's personal life in the real world, has not yet been considered.

This paper focuses on defining the concept of digital wellbeing, the requirements for its legislative anchoring or inclusion in company regulations, and introducing selected tools for maintaining digital wellbeing.

The paper is based on a search and analysis of mainly legislative documents and standards valid in the Czech Republic and the EU. The need for more precise anchoring of digital wellbeing was monitored in an international questionnaire survey and the obtained outputs were refined by in-depth interviews.

Neither the ISO 45 000 series nor other applicable legislative documents in the Czech Republic explicitly mention digital wellbeing. However, there are already several countries in the EU that have legislated the right to disconnect (one of the essential components of digital wellbeing). Maintaining digital wellbeing is therefore currently dependent on informal agreements or formalised policies that each company sets at its own discretion. Digital wellbeing is likely to be one of the areas of focus for OSH in the near future. It is therefore worthwhile to start addressing it in workplaces of all kinds, especially in positions where hybrid working is possible.

The paper draws on insights gained through work on the Erasmus+ project 2021-1-SK01KA220-HED-000032017.

VÝZKUM INFORMAČNÍCH POTŘEB VYBRANÝCH SKUPIN EXTERNÍCH STAKEHOLDERŮ PRO POSOUZENÍ REPUTACE CHEMICKÉHO PODNIKU

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Příspěvek vyzdvihuje důležitost cílené firemní komunikace vůči různým skupinám stakeholderů při vytváření pozitivní reputace podniků. Jsou prezentovány výsledky primárního kvantitativního výzkumu, jehož základním cílem bylo zjistit, jaké informace jsou pro veřejnost v roli různých skupin externích stakeholderů chemického podniku důležité pro posouzení reputace tohoto podniku a jaké informační kanály jsou pro respondenty pro získání těchto informací preferované. Výzkum byl připraven na základě rešerše odborné literatury mapující předpokládané zdroje či nástroje pro vytváření reputace podniků a také identifikující nejvyužívanější firemní komunikační kanály pro komunikaci podniku s veřejností. Šetření potvrdilo předpoklad, že se informační potřeby mezi různými zkoumanými skupinami externích stakeholderů liší. Výsledky výzkumu poskytují chemickým podnikům efektivní návod pro specifické cílení jejich komunikace na různé skupiny stakeholderů s využitím vhodných informací šířených jimi preferovanými informačními zdroji.

COLLABORATION IN ENHANCING THE SUSTAINABILITY OF PACKAGING FOR CONSUMER CHEMICAL PRODUCTS

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Introduction

Industrial enterprises, including those in the chemical industry, undertake various activities to enhance the sustainability of their operations. One area they focus on is packaging. Sustainability of packaging is improved through various means, such as changing packaging materials, shapes, or designs, as well as managing packaging inventory and replenishment methods. While these changes in packaging can be pursued independently, enhancing the efficiency of proposed changes is achievable through collaboration with stakeholders of the company, particularly packaging suppliers. Collaboration can be developed both at a strategic level, involving packaging design, and in the current procurement of packaging. This article explores the forms of collaboration currently practiced in both of these areas, specifically in relation to packaging for consumer chemical products.

Methodology

The article presents the results of qualitative research conducted in companies purchasing packaging for their own products, specifically consumer chemical products. The research was carried out through personal interviews based on a predefined questioning scenario. The study examined trends influencing packaging management, the packaging design process, as well as the forms, methods, and approaches used in packaging inventory replenishment.

Results

The article presents the findings of the qualitative research, focusing on the current forms and methods of collaboration between companies and their suppliers, both at the strategic and tactical-operational levels. The research results are compared with theoretical insights in this field, than areas of collaboration issues are identified and recommendations for improvement are proposed.

Conclusion

The research findings, conclusions drawn, and recommendations provided in the article can contribute to the enhancement of sustainable packaging for consumer chemical products.

UTILIZING MULTI-CRITERIA DECISION ANALYSIS FOR NATURAL GAS DEHYDRATION OPTIMIZATION

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Multi-Criteria Decision Analysis (MCDA) is a powerful tool for decision-making in industry due to its ability to consider multiple factors simultaneously, providing a more comprehensive and structured approach. MCDA allows decision-makers to systematically evaluate alternatives, weight their importance, and generate well-informed decisions. Additionally, MCDA provides a sensitivity analysis framework, enhancing risk management and strategic planning.

The paper focuses on using MCDA in the reconstruction of a natural gas (NG) dehydration unit that removes water through absorption using triethylene glycol (TEG) as a solvent. There is an effort to reduce CO_2 emissions and improve economic viability while regenerating TEG through either distillation or stripping. Our study presents four operating options for the system. The conventional method (CM) uses 1500 kg/h of TEG. Two additional methods enhanced by NG stripping reduce TEG consumption to 1000 kg/h. NG is stripped to reboiler (SRM) and Stahl column (SSM). By investing in a smaller column, TEG consumption can be further reduced by 500 kg/h in both SRM ($SRM_{TEG,500}$) and SSM ($SSM_{TEG,500}$). The methods are compared based on economic aspect quantified by the specific product price (SPP), environmental impact by evaluating Eco-indicator 99 (EI99), and flexibility for future possible higher mass flow of NG requirements.

If the main priority is economics, then SRM is the best-ranked option. $SSM_{TEG,500}$, on the other hand, has the lowest environmental impact and achieved the highest score in case of environmental priority. If there are no specific criteria preferences, CM is ranked as the best alternative followed by SRM and $SSM_{TEG,500}$ with a comparable rating. Changes in the price of utilities, or emission allowances did not have any impact on the final ranking of alternatives.

We acknowledge the financial support provided by Slovak Society of Chemical Engineering. This study was supported by the Slovak Research and Development Agency under contract no. APVV-18-0-134.

BRIDGING THE KNOWLEDGE GAP: ASSESSING COMPETENCIES AND SKILLS FOR TECHNICAL EMPLOYEES IN ECONOMIC AND MANAGEMENT SECTORS - A CASE STUDY OF CHEMICAL AND FOOD INDUSTRIES IN SLOVAKIA

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Úvod

This contribution aimed to determine the knowledge, abilities, and competency needed for employees in technical domains in the economy and management sector. The research concentrated on chemical production and the food business in Slovakia, monitoring three groups of employees: food production manager, chemical production manager, and operational section manager. These explorations are part of the research that is being carried out as part of the development of an innovative model of education at the technical university. Its findings are intended to help students develop a profile that will be more applicable in practice.

Metodika

The initial phase of the study focused on analyzing the essential competencies, professional knowledge, and skills needed for specific professions as outlined in state registers such as the National System of Occupations and National System of Qualifications. It also aimed to determine if university study programs in these fields have fully incorporated the requirements set by industry experts in management and economics.

The second phase of the study involved analyzing the needs of the business environment, with a specific focus on medium-sized enterprises in the food industry. We surveyed organizations with a turnover exceeding €50 million using a systematic questionnaire to determine their specific labor needs, particularly focusing on economic and managerial expertise requirements.

Výsledky

We discovered that while most fields we surveyed have these prerequisites in place, they are primarily voluntary, with just a small number of students opting for these subjects. Upon further examination, it was discovered that even in non-managerial fields such as chemical and food technology (technologist, specialist, technician), there are requirements for fundamental knowledge in economics and management in national registers. However, the number of individuals completing education in these areas at universities is minimal.

Over 32% of eligible food companies in Slovakia participated in the questionnaire. 43% of firms believe it is crucial for technically oriented individuals to possess fundamental understanding in economics, management, and marketing. The most commonly cited requirements were accounting, controlling, and budgeting. Employees prioritize past job experience, practice, education in the industry, personal impression, and assign the least significance for salary requirements.

Závěr

Our findings suggest a more integrated curriculum development method to ensure university study programs meet industrial standards. Our research shows that state registrations list critical competencies, but these requirements are generally considered as voluntary, resulting in few students choosing disciplines that bridge technical and managerial skills.The research found that universities need to deepen their collaboration in curriculum development with practice and their needs. This is evidenced by the gradual introduction of professional study programmes that are valued by practice and at the same time the experience gained in them is deepened during the study in practice.

This study was funded by project KEGA research task no. 011STU-4/2022 "Creating a model of education supporting the increase of competencies of students of a non-economically oriented university in the field of innovative, entrepreneurial thinking and business support" conducted at the Institute of Management of the STU in Bratislava.

POTENCIONÁLNE DOPADY ENVIRONMENTÁLNEHO VZDELÁVANIA NA ZELENÚ EKONOMIKU

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Úvod

Zelená ekonomika je ekonomika, podporujúca ľudskú prosperitu a sociálnu rovnosť za súčasného výrazného zníženia environmentálnych rizík a ekologických škôd. Školské vzdelávanie v obalsti odpadového hospodárstav s akcentom na vdoua vodné hospodárstvo má okrem jadnostliivca vplyv aj an priemsel. Chemický priemysel spotrebúváva veľké množstvo vody. Poster identifikuje potencionálne dopady vzdelávania na zvyšovanie kvality života a ich dopady na ekonomiku priemyslu.

Metodika

Predikovanie ekonomických dopadov na zvyšovanie kvality života a na priemysel (chemický).

Výsledky

Ekonomické zhodnotenie dopadov eko vzdelávanie na kvalitu života a priemysel

Závěr

Investovanie do oblasti vzdelávanie prináša okrem zvyšovania kvality života, lepšie hospodárenie s prírodnými zdrojmi aj na zvyšovanie efektivity priemyslu.

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HOW HOST AND HOME COUNTRY INSTITUTIONAL COMPLEXITIES INFLUENCES CSR ENGAGEMENT OF AN MNC: EVIDENCE FROM ESG DISCLOSURES OF A GERMAN MULTINATIONAL CHEMICAL COMPANY AND ITS INDIAN SUBSIDIARY.

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In this globalized free trade era, cross-border CSR engagements of multinational corporations have an overarching impact on societies, while ensuring their much-needed legitimacy in host and home markets. In international business and business ethics streams, many studies dealt with MNCs' responsibility practicesand the challenges associated with the institutional duality they must address when operating in environmentally dispersed markets with the same set of parental business values. A micro-level study that discusses a particular MNC's difference in CSR engagement within its home and host country is relatively scarce. This study is organized into two parts, the first critically examines the institutional complexities prevailing in Europe and the Indian business environment that shape specific CSR engagements and states a few propositions based on that. In the next part, we test the validity of those propositions by pitching them against real-life CSR business practice. We examine how institutional factors influence the CSR engagement of a chemical company from Germany that has a fully-owned subsidiary in India. Content analysis is employed on respective ESG reports released by the MNC on their global website and the subsidiary's Indian website. A visible pattern and prioritization in ESG disclosure were found in both reports, complementing the propositions. The German parent company prioritized climate control, employee rights and governance compared to its subsidiary in India, wherein the subsidiary gives more time, effort, and money to community development causes. This study provides practical CSR engagement insights for European chemical companies while operating in Indian markets.

Biotechnology and biorefinery

METHYLOMES OF *CALDIMONAS THERMODEPOLYMERANS* STUDIED WITH THE THIRD GENERATION SEQUENCING PLATFORMS

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Genus *Caldimonas* presents, after several reclassifications proposed during the last two years, a relatively diverse group of Gram-negative thermophilic bacteria. Special attention is paid to *C. thermodepolymerans* species due to its polyhydroxybutyrate-producing ability from xylose which is preferred by the bacterium over glucose. Only recently, we have finished besides the type strain *C. thermodepolymerans* DSM 15344^{T}'s also genomes of strains DSM 15264 and LMG 21645. Apart from minor differences in genome sequences, we captured relatively major differences in methylated sites. Unfortunately, using older Oxford Nanopore Technologies (ONT) Flow Cells R9.4.1 and chemistry did not allow us to infer methylated sites with sufficient accuracy. Therefore, we decided to perform resequencing of all three genomes with the newest ONT Flow Cells R10.4.1 and V14 chemistry allowing for much more accurate analysis. To further support the detection of methylated bases, we additionally used the Pacific Biosience (PacBio) Sequel IIe platform for additional resequencing. Finally, we combined methylations detected by both platforms while comparing epigenomes of particular strains.

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IMPAIRED SOLVENTOGENESIS AS A RESPONSE TO LIGNOCELLULOSE INHIBITORS IN ABE FERMENTATION

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ABE fermentation is a process that involves the production of solvents, namely acetone, butanol, and ethanol, by a group of anaerobic bacteria known as solventogenic clostridia. These bacteria were extensively utilized for industrial solvent production during the first half of the 20th century. With the advent of the petrochemical industry, biotechnology-based processes were not able to compete economically and nowadays there is no bulk biotechnological production of ABE in the World. Recent shifts in ecological priorities and a growing emphasis on sustainability have revived the potential for biotechnological ABE production. However, only waste or side streams are considered viable substrates. Lignocellulose biomass is a promising substrate option, but inhibitors released during its pretreatment negatively impact solvent production and final titers. Inhibitors' presence leads to an increase in acid production, causing media over-acidification, growth cessation, and cell death. Despite numerous hypotheses attempting to explain this phenomenon, none have been conclusively verified to date. Based on our collected data with the *Clostridium beijerinckii* NRRL B-598 strain, both with and without the addition of inhibitors, existing hypotheses will be discussed. Furthermore, a new hypothesis and potential solutions to mitigate the negative impact of inhibitors will be proposed.

This work was performed thanks to the financial support of the project GACR 23-06941S.

SUSTAINABLE *LIMNOSPIRA MAXIMA* (SPIRULINA) PHOTOAUTOTROPHIC CULTIVATION USING ARTIFICIAL LIGHT SOURCES: THE INFLUENCE OF LIGHT SPECTRA AND INTENSITY ON BIOMASS AND PIGMENT PRODUCTION AND COST

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Limnospira maxima is a cyanobacteria used as food and feed supplement and also as a source of antioxidants and pigments for food industry. It also, serves as a model organism for sustainable food production due to its high nutritional value and minimal environmental footprint. This study investigates the influence of light quality on *L. maxima* biomass and pigments production, such as c-phycocyanin, chlorophyll *a*, and carotenoids, with a focus on optimizing cost efficiency of cultivation process, considering the artificial illumination as the main operational cost. Series of experiments using different light intensities (20 – 550 μmol/m^2/s) and different light spectral composition (day white, warm white, red, yellow, green, and blue LED) were performed. The experiments revealed a clear correlation between light intensity and culture productivity, with higher intensities leading to increased biomass concentrations/productivity, in contrast, pigments content had a maximum at moderate intensities and decreased when the high intensities were applied. The dependence of biomass and pigment content and productivity on the different light spectra tested was much less straightforward. The interpretation of these results is rather complex due to their multiple outcomes. For instance, when the same light intensity of different spectra was applied, the content of carotenoids was the highest for blue light and the content of c-phycocyanin in all tested light colors did not show significant differences. However, in terms of biomass and pigments productivity, blue light showed the lowest values and therefore the highest energy and financial cost. In contrast, day and warm white lights were found to be the most effective for biomass productivity and the least effective for c-phycocyanin productivity and content, resulting in higher energy and financial costs. However, in terms of pigments content, blue light was certainly showing the best results. These findings provide information for optimizing biomass and pigment production considering economic perspectives. Therefore, they can contribute to the development of cost-effective and sustainable strategies for *L. maxima* cultivation.

STRESS CONDITIONS INFLUENCING THE PRODUCTION OF MONASCUS SECONDARY METABOLITES

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The *Monascus* fungi are ascomycetes known and used in Asian countries from ancient times. A wide variety of secondary metabolites are synthesized by the species within this genus, the most important are monacolins – the inhibitors of cholesterol synthesis, pigments and mycotoxin citrinin.

In this presented work, we studied the impact of different conditions on secondary metabolites production. Two monascal strains: *Monascus purpureus* DBM 4320 and *Monascus* sp. DBM 4361, were cultivated in liquid media containing different concentrations of NaCl and glucose. With the increasing salinity decreasing trends in growth and production of pigments and citrinin were observed in both strains. In the case of *Monascus purpureus* in the presence of both types of stressors, a smaller amount of biomass was determined and the glucose as the carbon source was not fully consumed. Unconsumed glucose was detected also at the second tested strain at the highest glucose concentration (150 g/L). *Monascus purpureus* strain produced manyfold larger amounts of secondary metabolites. In the presence of higher glucose concentrations, the aerobic production of ethanol occurred. In the cultivation of *Monascus* sp. in the presence of higher concentrations of NaCl, enhanced production of osmoprotective compound – glycerol was observed. And the correlation between stress conditions and increased production of mycotoxin citrinin has not been observed.

BACTERIA IN PLANT GROWTH PROMOTION AND PROTECTION

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The replacement of chemical fertilizers and pesticides and the transition to sustainable plant agriculture requires a deeper understanding of interspecies relationships in nature, including those between plants and microorganisms. Many plant-populating bacteria, called epi- and endophytes, can promote plant growth as well as prevent the development of plant diseases or prevent plant pests. The bacteria can thus be used in organic microbial pesticides, fungicides and fertilizers. Useful properties of bacteria in this sense are the production of enzymes such as chitinases, the formation of secondary metabolites inhibiting fungal growth, the ability to produce plant hormones, the solubilization of phosphates, the release of ammonium ions and others. The advantage of using bacteria is also their ability to grow on agricultural and food waste substrates such as brewery mash, whey, waste from animal production (feathers, meat separation residues, fish scales, etc.). These wastes, after relatively easy pretreatment by hydrolysis under mild conditions (no pressure, low acid or base concentration), can be used as a complex culture medium for bacteria. The composition of the culture medium and the setting of culture conditions can influence not only the growth of bacteria but also the production of desired metabolites and enzymes. After cultivation, the whole medium together with the bacteria can be used for application to plants. The concept of this bacterial utilization and at the same time waste valorization within circular economy will be demonstrated with the example of the endophytic bacterium *Pantoea agglomerans* DBM 3797, isolated from hops.

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EXTRACTS FROM PLANT MATERIALS AND EVALUATION OF THEIR BIOLOGICAL ACTIVITIES

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The aim of this contribution is a summary of the results and the methods used to measure the biological activities of extracts from selected plant materials.
Natural substances have been used historically, for example, in traditional medicine. Their main advantage is that they belong to easily renewable sources with a rich species representation and a wide spectrum of biologically active substances. However, many valuable properties of these substances remain undiscovered, or their effects remain unclear. Extracts from natural substances are therefore still the subject of current research.
The subject of the study was the preparation and testing of extracts from a total of 9 plant species (*Rosmarinus*, *Cupressus*, *Hippophae*, *Magnolia*, *Leuzea*, *Rhodiola*, *Trichilia*, *Eleuterococcus* and *Calendula*). Individual extracts were obtained using supercritical fluid extraction (SFE), pressurized liquid extraction (PLE), standardized Harborne extraction procedure of secondary metabolite, Soxhlet extraction, the two-phase extraction method or leaching and preparation of tinctures, decoctions and infusions. The obtained extracts were always evaluated by a battery of tests, based in principle on the determination of activities that could be used in the treatment of the most common human diseases, such as infectious or oncological diseases. Based on this assumption, the measurement of biological activities mainly included methods for determining antimicrobial, cytotoxic, anti-inflammatory, antioxidant, anti-diabetic, and acetylcholinesterase effects.
The conducted research summarizes and compares results from several years and presents the best candidates who can contribute to finding an effective plant species or biologically active substance with potential use in medicine.

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FROM WASTE TO WONDER: TRANSFORMING FEATHERS INTO NUTRIENTS USED FOR MICROBIAL CALCITE PRECIPITATION

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The construction sector is a significant contributor to greenhouse gas emissions, accounting for approximately 7% of worldwide CO_2 emissions. Among these emissions, the production of Portland cement represents the largest portion, at 80%. Consequently, there are numerous challenges associated with recycling and treating the waste generated during demolitions. In our previous experiments, we have identified that waste concrete fines (WCF) with a diameter smaller than 4.75 mm show promise for recycling through a biomineralization process known as microbially induced calcite precipitation (MICP). Our research has explored various parameters of the biomineralization process, including the concentration of bacterial cells, pH adjustments of WCF suspensions, and single or repeated injections of bacterial suspensions. We have assessed the cohesion of the formed composites and their mechanical properties (Holecek P. et al., 2024; Klikova K. et al., 2024).

To enhance the cost-effectiveness of this process and align with the principles of the circular economy, it is essential to find alternatives to commercial culture media. One promising option is the utilization of raw feathers from chicken slaughter, which can be efficiently hydrolyzed into soluble peptides (Stiborova et al., 2016). In this study, we have optimized the conditions for feather hydrolysis to develop feather hydrolysate as a substitute for commercial culture media. By utilizing Design of Experiment software, particularly StatEase, we have analyzed factors such as hydrolysis time and temperature, feather quantity, hydroxide concentration, and the proportion of yeast extract addition. Through Response Surface Analysis, we aim to determine the optimal composition for supporting the growth of bacterial strains involved in the biomineralization process. By implementing this cost-effective culture medium, we anticipate a reduction in the carbon footprint associated with economic and environmental requirements. This innovative approach not only offers a sustainable solution for waste recycling in the construction industry but also contributes to mitigating the environmental impact of construction activities.

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RECYCLING WASTE CONCRETE FINES USING MICROBIAL CALCITE PRECIPITATION VIA VARIOUS METABOLIC PATHWAYS

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Reducing the carbon footprint and recycling materials are the main goals of recent years, which have been confirmed by the approval of the Paris Climate Agreement in 2015. Global warming and climate change stand as significant challenges demanding collective attention and action across various sectors and societies. Cement production, integral to the construction industry, emerges as a significant contributor to anthropogenic CO_2 emissions worldwide, accounting for around 7-10% of the total emissions (Hanifa et al., 2023). One of the effective methods for reducing CO_2 emissions while recovering waste construction material (waste concrete fines – WCF) for reuse is by employing the MICP process.

In this study, we compared the efficacy of microbially induced calcite precipitation (MICP) using two distinct metabolic pathways (carbonic anhydrase and urease) involving different genera of bacteria (*Bacillus cohnii* DSM 6307 and *Sporosarcina pasteurii* DSM 33). We examined three types of waste concrete fines (WCF) characterized by differences in age, grain size distribution, and physical-chemical properties. Both bacterial types have the capability to form calcium carbonate crystals, and biocementation solution containing calcium ion and nutrients for their growth was added repeatedly within 30 days. Final analyses, including scanning electron microscopy (SEM), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), and mechanical property assessments for cohesiveness were evaluated for all samples.

In light of our results, it is apparent that the utilization of *Bacillus cohnii* DSM 6307 with carbonic anhydrase activity provides more compact composites with better mechanical properties as the result of MICP ability than the ureolytic bacterium *Sporosarcina pasteurii* DSM 33. Based on our findings, it can be concluded that MICP presents a promising method for recycling waste concrete fines as a way to reduce carbon footprint.

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THE PROPERTIES OF LAVENDER PAPER AS A POTENTIAL WASTE MATERIAL FOR PAPER PRODUCTION

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Nowadays, the emphasis is on the use of waste crops in the context of the circular economy and waste management. For this reason, waste lavender has been used for paper production. The main reason for using lavender as a raw material is that a large amount of waste stem remains after harvesting. This paper deals with the mechanical and physical properties. Tensile strength and burst strength were evaluated as the fundamental mechanical properties. At the same time, the physical property, namely Gurley air permeability, was also tested. This was mainly because of the resulting paper's resistance to the moth mall. Surprisingly, the highest strength values were achieved by the 80 $g \cdot m^{-2}$ paper with a breaking length of 1.71 km and a tensile strength of 16.76 $Nm \cdot g^{-1}$ compared to the higher basis weights of 100 and 120 $g \cdot m^{-2}$. In addition to the properties of the finished paper, the feedstock was analyzed for its chemical components. The results of this research show lavender waste as another potential raw material for paper production.

DETERMINATION OF THE PROPERTIES OF COTTON PULP WITH THE ADDITION OF NANOCELLULOSE

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Nanocellulose application is an emerging field of study. This study aimed to apply nanocellulose to special paper products. For those purposes, beaten and unbeaten cotton pulp properties were determined with and without the addition of nanocellulose. Cotton is commonly used for special paper products because of its long fibers. Therefore it is interesting to investigate its properties for special purposes. In this research, tensile properties and burst index were evaluated for mechanical properties. For physical properties, Gurley air permeability was tested. Optical measurements were evaluated to assess the whiteness of paper samples. The tensile index for unbeaten cotton pulp without nanocellulose was on average 5.22 Nm/g and with 1% NC addition 9.05 Nm/g with a 73.37% increase. Same property, the tensile index for beaten cotton without nanocellulose was on average 18.23 Nm/g and with 1% NC addition 20.46 Nm/g with a 12.23% increase. Therefore, the determination of properties evaluated in this paper can be used for special paper products from cotton pulp.

THE DEVELOPMENT OF THE ANALYTICAL PROFILES OF FRUIT DISTILLATES DURING THE DISTILLATION PROCESS

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Fruit distillates, also known as fruit spirits, are alcoholic beverages with a rich cultural heritage and various production techniques around the world. The production process of fruit spirits consists of the selection of quality raw materials, fermenting the fruit mash and then separating the volatile compounds by distillation. During the production process there are many factors that can affect the quality of the resulting distillate and one of the key factors is the execution of the distillation. The fractions at the beginning of the distillation, known as the “head“ fraction, and at the end of the distillation, known as the “tail“ fraction, carry undesirable organoleptic characteristics and are therefore usually separated from so-called “heart“ fraction, which is collected. Distillers try to optimise the distillation process to maximise the ethanol yield while minimising the concentration of undesirable compounds. The aim of this work was to study the evolution of the analytical profiles of distillates flowing from the alembic during distillation and to identify compounds that are preferentially present at the beginning or end of distillation and their concentration in the distillates can be therefore controlled by adjusting amounts of both separated franctions. With the use of sensory analysis, it will then be possible to determine the positive or negative influence of these substances on the organoleptic properties of distilled spirits and to determine their optimal concentration in these beverages, towards which the distillation process can be directed.

THE IMPACT OF HYDROGEL BIOINOCULANTS IN PLANT RESISTANCE TO DROUGHT CONDITIONS

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Climate change has a significant influence on an agricultural production worldwide. Watering of plants and crops is essential and desirable, nevertheless consistent high temperatures demand careful monitoring and optimization of irrigation practices to mitigate water loss and maintain crop yields. One potential solution for retaining water could be the implementation of hydrogels with encapsulated plant-growth promoting bacteria (PGPR).

Azotobacter vinelandii belongs to PGPR and shows biological activities for the stimulation of plant growth and is capable of synthesizing two completely different biopolymers with great application potential. Polyhydroxyalkanoates (PHA) are produced and stored in the form of intracellular granules improving cell robustness, while alginate is produced extracellularly and used for bacterial protection.

In this work, hydrogels with encapsulated bacteria, by direct gelation of bacterial alginate, are formed and employed into the soil with lettuce seeds. After 40 days of plant grow, we stopped watering the plants and observed how the plants were influenced by drought. The experiment showed positive results not only in the improved condition of plants (including higher biomass and increased content of both plants and roots), but also in higher resistance to drought in treated plants compared to untreated ones.

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THE USE OF HYDROLYSATES MADE FROM FOOD INDUSTRY WASTE AS CULTURE MEDIUM FOR ENDOPHYTIC MICROORGANISMS

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The food industry produces large amounts of unwanted waste that could still be used in other industries. Organic food wastes such as feathers, meat, plants, but also yeast from breweries can be easily converted into hydrolysates, leading to their use in cultivation as a substrate for microorganisms such as endophytic bacteria in this project. Bacteria are able to grow better in these types of complex media compared to the well-known non-sugar LB medium (Luria Bretani lysogeny broth) and due to the high peptide content, hundreds of miligrams per liter of ammonium ions are released through bacterial metabolism mostly as their unused nitrogen source. Other advantages of some of these bacteria include the ability to produce secondary metabolites such as indole-3-acetic acid and to perform phosphate solubilization, which is one of the desirable characteristics of applied microorganisms for plant growth promotion, commonly known as Growth Promoting Activity. When all these properties are combined, it is an opportunity to prepare a biofertilizer that could be used in agriculture. This whole process is one example of the so-called circular economy.

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SMALL RNA ANALYSIS IN CALDIMONAS THERMODEPOLYMERANS PROVIDES INSIGHT INTO NON-CODING REGULATORY MECHANISMS

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Caldimonas thermodepolymerans DSM 15344^T is a non-model thermophilic bacterium producing polyhydroxyalkanoates (PHA), biodegradable and biocompatible alternatives to petrochemical plastics. The synthesis of these polymers in bacteria is known, in most cases, to occur under stress conditions such as stress caused by nutrient limitation. Similarly, small RNAs (sRNAs) are closely linked to stress conditions. These regulatory molecules are known to be involved in post-transcriptional regulatory processes. They are predominantly induced in response to stress and further interact with mRNA molecules to impact their translation into functional units. Such common characteristic suggests a possible regulation of the PHA synthesis pathway by sRNAs and thus extends the potential of bacteria for biotechnological applications. Even though many sRNAs have been found and reported, yet there is still lack of sRNA annotations. Here we present results from downstream analysis of RNA-Seq data from xylose cultivation up to 72h covering 8 time points, each in 3 biological replicates. Following sRNA inference, we performed differential expression analysis and co-expression analysis using state-of-the-art tools. These results provide deeper insight into regulatory mechanism of *C. thermodepolymerans* with the introduction of candidate sRNAs and their expression profiles, further used for the guilt-by-association functional annotation.

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CULTIVATION OF CAROTENOGENIC YEAST ON VARIOUS FOOD INDUSTRIAL WASTE SUBSTRATES

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Carotenogenic yeasts are a group of yeasts that produce orange to red pigments in the form of carotenoids. They are also known for their ability to produce a significant amount of other bioactive substances, including ubiquinone, ergosterol, betaglucans, proteins and lipids. Their great biotechnological potential lies in the ability of utilizing many waste materials to produce biomass enriched by the bioactive substances under the biorefinery concept. The adaptability of carotenogenic yeasts allows them to use different waste substrates for their growth, e.g. oils and fats, chicken feather hydrolysate, lignocellulose materials and many others. Specifically, this study focuses on combined utilization of whey, waste poultry fat and waste frying oil as nutrition sources.

In this study, the yeast strains *Rhodotorula toruloides* and *Cystofilobasidium macerans* were studied. Batch cultivations were carried out in artificial media with the addition of waste substrates at different C/N ratios. In these experiments, the best yield was achieved by the strain *Cystofilobasidium macerans* on waste whey with the biomass yield 21.65 g/l. The strain *Rhodotorula toruloides* achieved an increased yield of biomass (14.35 g/l) on glycerol, which can serve as a model for waste glycerol obtained from biofuel production. The main goal of future research is to test also other red yeast strains such as *Phaffia* sp. and *Sporidiobolus* sp. in the presence of waste substrates and to scale-up these cultivations to the laboratory bioreactor.

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SYNTHESIZING POLYHYDROXYALKANOATES FROM WHEAT BRAN HYDROLYSATES VIA HALOPHILIC BACTERIA

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Dealing with the increasing amount of waste from the food industry is a big problem worldwide. Lignocellulosic materials are a type of this waste. They can be used in different ways, like making biofuel, creating chemicals, and producing biodegradable plastics called polyhydroxyalkanoates (PHAs). PHAs are biodegradable, and biocompatible, and can be generated from renewable resources as intracellular granules by various prokaryotic microorganisms.

Lignocellulosic materials are made up of cellulose, hemicellulose, and lignin. By chemical and biochemical pretreatment, these materials can be hydrolysed to obtain fractions suitable for the synthesis of valuable compounds. Cellulose and hemicellulose can be broken down by high-pressure and thermal pretreatment and enzymatic hydrolysis into monosaccharides that serve as a carbon source for bacteria capable of producing PHA. The use of lignocellulose-based resources as a substrate for PHA production represents an opportunity to reduce production costs.

In this research, we analyzed the composition of wheat bran hydrolysates obtained through a combination of chemical and enzymatic hydrolysis. The hydrolysates were evaluated mainly concerning the concentration of reducing saccharides. Subsequently, we cultivated two specific strains of halophilic bacteria, namely *Halomonas halophila* CCM 3662 and *Halomonas organivorans* CCM 7142T, using these hydrolysates. Firstly, we cultivated these two bacterial strains in flasks and then we scaled up the process to laboratory bioreactors (batch cultivations). We determined the production of polyhydroxyalkanoates (PHAs) by gas chromatography with a flame ionization detector. *Halomonas halophila* showed the highest PHA production in flasks, 2.5 ±0.1 g/L, which represented approximately 68 % of the dry cell weight. However, *Halomonas organivorans* achieved a higher PHA yield of 3.8 ±0.1 g/l when cultured in bioreactors, which represented approximately 37 % of the dry cell weight.

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CULTIVATION OF CLOSTRIDIUM BUTYRICUM ON LIMNOSPIRA MAXIMA SUBSTRATES

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Probiotics, live microorganisms ingested through food or supplementation, have the ability to improve gut microbiota balance and exert positive effects on host health through wide range of action modes. *Clostridium butyricum* (CB) is a spore forming anaerobic bacteria which is beneficial in management and treatment of digestive tract diseases, increasing resistance to pathogens and modulating immune response. Cultivation of CB on nutrient rich substrates, which support bacterial growth due to presence of prebiotic compounds, may provide added value to probiotic supplement nutrient content, viability and resistance of spores after consumption.

This work investigates the possibility of cultivation of CB on *Limnospira maxima* (Spirulina), a food-grade algae, as a replacement of conventional complex nitrogen sources in media. Spirulina, rich in bioactive compounds, protein and oligosaccharides, will be treated by various mechanical methods of cell disruption, in order to preserve integrity of bioactive compounds while making the intracellular nutrients, primarily nitrogen sources, more available for CB. CB growth and spore production on spirulina after mechanical treatments will be assessed in comparison to conventional complex nitrogen sources, expressed as maximum growth and maximum sporulation.

Project anticipates overall successful cultivation of CB on spirulina substrates, as well as different cell growth dynamics after various cell disruption methods.

Successful cultivation may yield a product with a superior nutrient profile, improved bioavailability of bioactive compounds, and enhanced viability of CB. This approach could address the challenges associated with fresh spirulina consumption such as short shelf life, and improve the quality of probiotic preparate. The findings may contribute to the development of nutritionally enriched probiotics, fostering advancements in probiotic biotechnology.

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IMPACT OF FERULIC AND COUMARIC ACIDS ON SOLVENTOGENIC CLOSTRIDIA

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Cultivation of solventogenic clostridia on lignocellulosic biomass represents a promising way for sustainable bio-solvents production. Lignocellulosic biomass serves as an ideal substrate for clostridia due to its rich content of cellulose. However, the dense and complex structure of lignocellulose requires a pretreatment to improve its accessibility. Once pretreated, the biomass can be fermented by solventogenic clostridia through process known as ABE fermentation, where solvents like acetone, butanol, and ethanol are produced. However, during pretreatment, inhibitory compounds such as ferulic and coumaric acids are released, inhibiting the growth of solventogenic clostridia and affecting their ability to produce solvents. The objective of this research was to explore the effect of ferulic and coumaric acids on solvent production during the cultivation of *Clostridium beijerinckii* NRRL B-598. When a combination of ferulic and coumaric acids (0,2 g/l each) was added during batch cultivation, there was an increase in acid production coupled with decrease in solvent production. Thus, the culture did not switch from acidogenic to solventogenic phase under these conditions. Nevertheless, during fed-batch cultivation, where the same concentration of inhibitors was added to the medium gradually, solvent production remained unaffected. Finally, the resulting solvent concentration in the culture exposed to inhibitors did not significantly differ from the control culture devoid of inhibitors.

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APPLICATION OF EXTRACTIVE BIOTRANSFORMATION IN SYSTEM OF TWO COUPLED MEMBRANE BIOREACTORS

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During the bioproduction of substances using microorganisms the strong product inhibition can occur which dramatically decrease the efficiency of the process. To overcome this an in-situ removal of the product from the fermentation medium is necessary to apply. One way how to do it is to use membrane separation connected with bioproduction in bioreactor to one unit, membrane bioreactor.

Some of the natural substances are impossible to produce directly using one strain of microorganism and they must be produced via one or more intermediates requiring the use of different production strain for each one. Good example is the bioproduction of phenylacetaldehyde from 2-phenylethanol by the bacteria *Gluconobacter oxydans* and the biotransformation of L-phenylalanine to 2-phenylethanol biocatalysed by yeasts *Saccharomyces cerevisiae*. Both, phenylacetaldehyde and 2-phenylethanol are products inhibiting the biotransformation.

In this work the bioproduction of phenylacetaldehyde directly from the substrate L-phenylalanine through the intermediate 2-phenylethanol is presented. Bioproduction is performed in the system of two interconnected membrane bioreactors containing different production strains with membrane separation based on pertraction and membrane extraction and linked with regeneration unit where product is accumulated. This configuration leads to high level of integration and intensification of the production process.

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BIOINFORMATICS ANALYSIS OF *CALDIMONAS'* ABILITY FOR BIOTRANSFORMATION OF FERULIC ACID INTO VALUABLE PRODUCTS

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Caldimonas thermodepolymerans (formerly *Schlegellela thermodepolymerans*), an aerobic, gram-negative thermophilic bacterium, exhibits remarkable biotechnological potential in its ability to biotransform ferulic acid into high-value metabolites. This study is devoted to the bacterium's proficiency in the conversion of ferulic acid into vanillyl alcohol and vanillic acid.

Through genomic analysis of *C. thermodepolymerans* strains DSM 15344^T, DSM 15264, and LMG 21645^T, several putative genes encoding enzymes involved in ferulic acid metabolism were identified. Specifically, the gene *fcs* (KO number K12508), encoding feruloyl-CoA synthase, was identified in all three analyzed genomes. Although the gene *ech* (K07511), encoding enoyl-CoA hydratase/aldolase, was not directly annotated, its presence was inferred based on its co-localization with *fcs* in the same operon. Gene *aat* (K00684), encoding leucyl/phenylalanyl-tRNA protein transferase, was also identified in all analyzed genomes. However, the putative *vdh* gene encoding vanillin dehydrogenase could not be identified yet, probably due to its low genomic sequence homology with species known to contain the vanillin dehydrogenase gene.

Furthermore, a comparison with other *Caldimonas* species, particularly *C. aquatica*, revealed that only *C. thermodepolymerans* possesses the genetic information necessary for ferulic acid biotransformation. These findings underscore the unique biotechnological potential of *C. thermodepolymerans* within the *Caldimonas* genus.

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THE WINE INDUSTRY BY-PRODUCTS: ANTIBACTERIAL & PREBIOTIC ACTIVITY OF EXTRACTS IN RELATION TO TOTAL PHENOLIC COMPOUNDS

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The waste materials generated by the wine industry, often overlooked and neglected, possess significant potential for extensive pharmaceutical and food applications. By-products of grape processing, such as grape pomace, stems, and canes, represent valuable reservoirs of bioactive compounds, particularly polyphenols. Polyphenols have garnered increasing scientific interest due to their diverse potential health benefits, including their impact on the human microbiome.

This study focused on assessing the influence of polyphenols, extracted from *Vitis vinifera* processing by-products, on specific bacteria relevant to the human digestive system. This study aimed on the prebiotic and antibiotic effects of *Vitis vinifera* extracts on bacterial representatives of the gut microbiota, both in suspension and in biofilm. Ethanolic extracts from *Vitis vinifera* pomace, stems and canes were prepared, characterized and their effect on the biofilm formation was observed. The metabolic activity of biofilm cells was evaluated by the MTT viability assay.

Depending on the bacterial strain, the effect of extracts from pomace, stems and canes varied when applied on both planktonic and biofilm cells. Overall, the polyphenol supplementation stimulated the biofilm formation of the probiotic strains but inhibited the opportunistic pathogenic species. By applying *Vitis vinifera* extract at a concentration of 900 mgGA/L of total polyphenols, the metabolic activity of biofilm cells of all opportunistic pathogens was reduced by at least 50 %, while the probiotic strains were not negatively affected by same concentration.

This work highlights the complex potential of *Vitis vinifera* by-products in combating microbial pathogen growth and/or support the growth of probiotic bacteria, depended on the type of extract and its polyphenol composition.

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FEATHER HYDROLYSATE AS A COST-EFFECTIVE CULTURE MEDIUM FOR MICROBIAL-INDUCED CALCITE PRECIPITATION

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Climate change poses a significant threat to our planet, and initiatives such as the Green Deal are dedicated to mitigating its effects by focusing on the reduction of CO_2 emissions. A critical contributor to global CO_2 emissions is the construction industry, responsible for 5–10% of the total. Cement production, essential for concrete manufacturing, has a significant carbon footprint. However, innovative approaches, such as waste concrete fines (WCF) recycling and the production of bioconcrete through microbially induced calcite precipitation (MICP), offer promising solutions. Nevertheless, one of the primary challenges in implementing this technology is its cost, with the commercial culture medium constituting a considerable part of the overall expense. In this study, we investigate replacing commercial culture medium for two bacterial strains capable of MICP – *Sporosarcina pasteurii* (DSM 33) and *Bacillus cohnii* (DSM 6307) with waste feather hydrolysate as a cost-effective protein source. Using Design of Experiment software, specifically StatEase, we optimized the feather hydrolysis process for bacterial growth by exploring the following conditions: hydrolysis time, temperature, feather concentration, hydroxide concentration and yeast extract concentration. Applying the optimized conditions, according to the Response surface analysis, the feather hydrolysate can replace up to 90% of the commercial medium. Using this cost-effective culture medium, we prepared composite samples of bioconcrete. Preliminary results indicate that the strength of these samples is comparable to those using commercial media. These promising findings have the potential to significantly enhance the scalability and economic viability of the sustainable recycling of waste concrete fines.

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STUDY OF THE EFFECT OF ADAPTATION TO CONTINUOUS OSMOTIC STRESS ON THE BACTERIUM *RHODOSPIRILLUM RUBRUM*

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In recent years, there have been major advances in industry which, in addition to improving the quality of everyday life, has also caused massive enviromental pollution (e.g. plastic pollution). This issue could be solved by replacing the petrochemical plastics by in nature biodegrable materials such as polyhydroxyalkanoates (PHAs) also produced by purple non-sulfur bacterium *Rhodospirillum rubrum*. The advantage of this bacterium as a PHA producer is its metabolic versatility and thus its ability to survive in various conditions (light, dark, anaerobic or aerobic conditions, etc.). This work focused on the adaptation of *R. rubrum* to osmotic stress by evolutionary engineering with the goal of increased PHA production. First, the bacterial strain was exposed to different salt concentrations in order to optimize the appropriate salt concentration for subsequent adaptation experiment. During the evolutionary experiments, the PHA content of the adapted strains was analyzed by GC-FID, and the total dry biomass was also determined. After the evolutionary experiments, the cultures were exposed to selected stressors (high temperature; osmotic shock and freezing-thawing cycles) followed by viability analysis of by flow cytometry. We were able to confirm the positive effect of continuous exposure to osmotic stress of 40 g/l NaCl on PHA production in *R. rubrum* with the concentration of 15–20 % throughout the experiment. The method of evolutionary engineering seems to be appropriate for increasing PHA production in *R. rubrum*. In the future, it would be worthwhile to extend this work by including adaptations to other stressors in combination with carbon substrates other than those used in this work.

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MULTIPARAMETRIC OPTIMIZATION OF OPERATING CONDITIONS OF A MEMBRANE HYBRID SYSTEM FOR PHENYLACETALDEHYDE PRODUCTION

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Phenylacetaldehyde is an aromatic compound sourced from various fruits, honey, tea, and coffee. Apart from extraction from natural sources, it can also be obtained through biotransformation from L-phenylalanine in the presence of microorganisms, leading to the formation of the intermediate product 2-phenylethanol. In our case, *Saccharomyces cerevisiae* yeast was used for production of 2-phenylethanol, and for production of phenylacetaldehyde bacteria *Gluconobacter oxydans* was used. However, during production, the resulting products can cause inhibition of biotransformation. Continuous removal of the product can prevent this issue, creating a hybrid system where a membrane module is used for the extraction of 2-phenylethanol and phenylacetaldehyde. The aim of this work is the multi-parametric optimization of operating conditions of the membrane hybrid system with a focus on economy. The optimized membrane hybrid system consists of two bioreactors interconnected with pertraction and external extraction membrane modules to ensure continuous removal of 2-phenylethanol and phenylacetaldehyde. Creation of the mathematical model of the hybrid system and the process optimization was performed using MATLAB programming environment.

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ANIMAL WASTE AND ITS PROCESSING

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An alternative foodstuff such as insects is a very promising raw material not only for high content of proteins, but also for other nutritionally valuable components. Its advantage lays in the gentleness of breeding in relation to the environment. Its consumption is increasing similarly to the consumption of fish products. In addition, waste material from these productions containing amino acids, peptides, etc. has considerable potential as a secondary raw material that can be used, for example, in plant production. In addition to insect, waste materials from animal sources namely mealybug, carp (whole fish, fish remains), chicken (feathers, cartilage, meat remains) were tested in this study.
Hydrolysis of animal waste was carried out in a stirred stainless steel autoclave at a constant temperature of 140 °C for 5 hours. The experiments were carried out under slightly increased pressure in an inert atmosphere. The actual hydrolysis of protein components and lipids was initiated by a small addition of malic acid. After cooling, the reaction mixture was filtered on a batch vacuum device.
The solid residue of most tested raw materials represents a maximum of 5%. However, it can also be used as an admixture to plant residues for the preparation of high-quality vermicompost. The only exception is the solid shells of beetles, which cannot be completely decomposed under mild hydrolytic conditions. However, the outer solid skeleton is a valuable source of chitin, which (already as a pure source) is suitable for obtaining pure chitosan, used as a dietary supplement to eliminate fats in the human body.
Hydrolysates prepared in this way have the potential not only for use in agriculture as fertilizer or spraying on leaves to prevent excessive evaporation of water from plants and to supply nutrition. Last but not least, also as a biostimulation of soil bacteria, where it was experimentally found that the application of hydrolysates to the soil demonstrably increases the number of bacteria by at least 3 orders of magnitude.

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TWO IS BETTER THAN ONE – LINKING OF THERMOPHILIC BACTERIA TO ENHANCE PHA PRODUCTION

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Plastics are an essential part of our daily lives and almost everything that surrounds us. However, their ever-increasing production brings many negatives, particularly in the form of pollution, which has become one of the major environmental problems of our time and is beyond the nature's capacity to cope with. One approach is to try replacing part of petrochemical plastics with biobased and/or biodegradable plastics, both of which are met in microbial polyesters – polyhydroxyalkanoates (PHA). The biggest drawback, however, is the high cost of production, the reduction of which has become the mission of many scientists. Using thermophilic strains of bacteria as producers is a promising option. One of the adepts who have great potential in this field are the thermophilic bacteria of the genus *Aneurinibacillus*, which have recently been identified by our group as significant producers of unique PHA copolymers revealing extraordinary material properties. Another and no less interesting contender is *Caldimonas thermodepolymerans*, a moderately thermophilic bacteria that is capable of accumulating a significant amount of poly3-hydroxybutyrate P(3HB) from lignocellulose relevant sugars. Since both bacteria are very interesting and promising, but at the same time not thriving in a certain area, we aim to link these two worlds, especially from the context of knowledge in the field of molecular biology and genetics. In this way, we would create a perfect combination of two microorganisms, where the chassis would be *C. thermodepolymerans* enriched with a flexible synthetic device from *Aneurinibacillus* sp., thus achieving the production of interesting PHA copolymers even from inexpensive feedstocks. PHA production could be then introduced into the industrial sphere and compete with petrochemical plastics or join a very desirable field in biomedicine.

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KINETIC PERSPECTIVE ON BIODEGRADABLE PLASTICS DEGRADABILITY

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Since the age of plastics is under way, biodegradable plastics are gaining great popularity. Not only public promote these substituents of oil-based plastics, but a huge scientific interest was also attracted and further triggered an avalanche of praising and opposing studies. For instance, biodegradable polymers such as poly(lactic acid) (PLA) or polyhydroxyalkanoates (PHA) are intensively investigated from different perspectives in order to consider its suitability for commercial plastics replacement. There were several studies of accusing these biodegradable plastics of microplastics release and harming natural environments. Although common consumers put still higher demands on the environmental friendliness of purchased products, the end-of-life fate of the biodegradable plastics is still poorly understood.

In this study, we have investigated the biodegradation of commercial polyhydroxybutyrate (PHB) and PLA under thermophilic composting conditions from the kinetic perspective. Two different kinetic models have been applied to analyse the differences in the degradation mechanism – reaction order kinetics and release kinetics model. Evident differences in the degradation rate constants have been observed and together with SEM micrographs indicate different ways of degradation for PHB and PLA under thermophilic composting conditions. The results of this study highlight the necessity to deal with genuine biodegradability of plastics and to distinguish plastics generating durable microplastics from those truly biodegradable.

Gas Coal Fuel

BENEFITS OF AN OPTIMAL-SIZED COMBINED HEAT AND POWER PLANT FOR AN INDUSTRIAL ENTERPRISE

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Heat and electric energy are needed in every part of the industry. Nowadays, heat in the form of steam is usually being generated in a standard steam boiler, by combusting natural gas, while electricity is being purchased from the grid. But the ever-rising prices of energy, fuels and emission taxes are pushing enterprises to find a better solution. One of those can be the implementation of a cogeneration plant, which consists of a gas turbine, firing natural gas, that generates electricity and a heat recovery steam generator that utilizes waste heat from the turbine flue gas to generate steam. Produced steam can be used as a heating medium in the process, or to feed a steam turbine to generate even more electricity. This approach is more effective than the production of steam and electricity in two separate processes. Because of high efficiencies of modern turbines, and utilization of waste heat, using a cogeneration power plant can significantly reduce the amount of fuel burnt, and thus emissions generated, which benefits both the environment and the economy of the enterprise. This contribution focuses on the energy, environmental and economic comparison of installing and operating a standard steam boiler and a cogeneration plant, both in design and off-design conditions in an industrial enterprise. This work was supported by the Slovak Research and Development Agency, Grant No. APVV-18-0134. We also acknowledge the financial support provided by Slovak Society of Chemical Engineering.