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Decarbonisation and Economic Aspects of the Transformation of the Chemical Industry

- Decarbonisation – energy intensity, carbon capture and use
- Economics of the chemical industry in the new environment
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PLENARY LECTURES

THE SUN AND NANOMATERIALS FOR THE USAGEE OF CO_2, H_2O, N_2

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The increase in CO_2 in the atmosphere due to emissions is generally considered to be one of the main causes of global climate change. The main sources of CO_2 caused by human activity will be presented in the presentation. CO_2 is an easily and everywhere available gas that can be taken directly from the air. It is released during many industrial productions, in the energy sector, etc. CO_2 is used in a number of applications (e.g. chemical reactions, refrigeration, food industry). The dominant part of CO_2 is assimilated in green plants during photosynthesis. However, plants are not able to "process" all the excess CO_2.

In this contribution, the possibility of using "airy" CO_2 for (i) the preparation of monomers for the next polymers synthesis will be discussed. When using "green" hydrogen, CO_2 can be used also for (ii) the production of hydrocarbons (so-called e-diesel) and methanol. Next, we will focus on "artificial photosynthesis", which can be prepared directly from methanol. Furthermore, the possibility of preparing H_2 using plasmon-stimulated **H_2O** splitting, its storage in COF structures and the use of plasmons in fuel cells will be discussed. As the next part of presentation the photocatalytic preparation of ammonia from atmospheric N_2 will be also described. All reactions, the use of "air" CO_2 for the preparation of polymers, the preparation of "green" hydrogen and ammonia, the preparation of methanol by "artificial photosynthesis" and the activation of fuel cells, are stimulated by the Sun on the nanostructures prepared by our team.

INORGANIC TECHNOLOGY

ANALYSIS OF SELECTED PROPERTIES OF HYDROXYAPATITE POWDER FOR THE PRODUCTION OF GRANULATE USED FOR FILAMENT FOR 3D PRINTING

Peciar P.[1], Jezsó K.[1], Guštafík A.[1], Úradníček J.[1], Veteška P.[2], Bača Ľ.[2], Thurzo A.[3], Janek M.[2]

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The application of 3D printing is a currently used process by which it is possible to make a part of the exact desired shape. Commonly commercially available applications and materials for 3D printing are easy to use. In the case of special applications, it is necessary to focus not only on the selection of the raw material, but also on individual processes that will affect the desired shape and properties of the product.

Among such special operations of 3D printing is use, for example, in dentistry. The special material used for 3D printing is ceramic - hydroxyapatite (HAP) in the form of powder, from which the filament is made by extrusion. The first step in the filament manufacturing process is the analysis of selected properties of the particulate material, such as particle size distribution, powder compressibility and flow functions.

Three different powder materials of hydroxyapatite (HAP) were used for further research application. Such an analysis predetermines the behaviour of the material in the extruder with the aim of creating a homogeneous filament for further processing.

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MINERAL FERTILIZER WITH NATURAL ANHYDRITE - CONNECTION OF LABORATORY AND PRODUCTION PRACTICE

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Controlled nutrition of plants consists in systematical replacement of mineral substances necessary for the healthy development of crops in the soil. Industrial fertilizers should help to balance and maintain the equilibrium of nutrients in the soil, possibly in plants. The elements used in plant nutrition are called biogenic. Main nutrients, or macroelements, are considered as essential in the cultivation of agricultural crops[1].

These include sulphur, which is present in all crops and plays an important metabolic role. It is essential for the formation of proteins, amino acids, vitamins and enzymes. It supports the creation of specific substances with influence on the taste, smell, aroma and by this also the specific properties of plants and plant products. Sulphur is becoming an increasingly important nutrient due to the combination of lower sulphur emissions, the increasing prevalence of fertilizers and higher cropping intensity.

The form of sulphates is the most accessible source of sulfur in the soil for plants. Sulphates enter to the metabolism of plants already in the roots or they are transported to the leaves, where, together with nitrogen, participate in the formation of proteins. Increasing of winter resistance and drought tolerance are other positive properties of sulphur-containing fertilizers. Leguminous plants, oilseeds, plants from the cabbage-family, hops, onions and root crops have the greatest requirements for sulphur[2,3].

One of sulphates applied to granular fertilizers, that serve as a source of sulphur, is calcium sulphate. The raw material for the future fertilizer with a content of 24% N and 6% S is anhydrite, anhydrous calcium sulphate – a natural raw material from Gemerská Hôrka.

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THE STABILITY MONITORING OF SOLID FERRATES(VI)

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The surface and groundwater water are currently polluted by different pollutants (pharmaceuticals, detergents, pesticides). The suitable option for wastewater treatment is the application of ferrates.

Ferrates $(FeO_4)^{2-}$ are compounds of iron in the high-oxidation state +VI. They are solid crystalline substances with a characteristic dark purple color. Ferrates are not only powerful oxidizing agents, but also an excellent disinfecting and coagulating agent. There are no carcinogenic or toxic products by their decomposition. These substances have high reactivity but relatively low stability. It is not possible to store them for a long time because of the decrease in purity.

The possibilities of increasing their stability, especially by different methods of encapsulation, are currently being investigated. Zeolites are a suitable material for encapsulation. Due to their porous structure, they appear to be an excellent sorption and filtration material. These substances have proven to be extremely effective in the treatment of wastewater for selective groups of contaminants. In addition, they are a natural and non-toxic material.

In this paper, we have monitored the stability of electrochemically prepared potassium ferrate. Ferrates were in the form of powder. In the experiment, ferrates with different purity (21.4 %, 63.5 % and 67.3 %) were used. They were encapsulated in packaging materials printed on a 3D printer. Different types of filaments were used (PVA, PLA, PVA+, and BVOH). The stability of the ferrate was monitored for three months. Different storage conditions of the ferrate samples were also compared. The storage conditions had a significant influence on the stability of the ferrate.

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INTRINSIC NATURE AND ACTIVE SURFACE SITES AFFECTING THE EFFECTIVITY OF Ni-Fe-W CATALYST

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Zero-gap alkaline water electrolysis (AWE) in combination with renewable energy sources represents promising technology for producing green hydrogen. The efficiency of zero-gap AWE can be increased by a suitable catalyst. Nickel and nickel-based materials have gained much attention due to their high potential as an effective catalyst. These materials can be easily prepared by electrodeposition. Important role in the effectivity of catalyst is played by active surface sites and intrinsic activity. Intrinsic activity of the catalyst depends on surface metal composition, the association of the metals concerned and the roughness of the surface. Active sites can be determined by ECSA (electrochemically active surface area) analysis. The aim of this work was to study multicomponent nickel-based catalysts prepared by electrodeposition. Combination of nickel, tungsten and iron was applied.

Ni-Fe-W coatings on nickel foam were prepared by electrodeposition on nickel foam substrate. Electrodeposition parameters such as current density of electrodeposition and composition of electrolyte were optimized to prepare catalyst with different composition and morphology. The prepared catalysts were characterised by means of SEM, XRD and EDX. Efficiency of the catalysts was investigated in a zero-gap electrolyser for AWE. ECSA of the catalysts was evaluated by cyclic voltammetry.

It was found that intrinsic nature of the catalyst influence effectivity of Ni-Fe-W catalyst. Ni-Fe-W catalyst with the highest iron content achieved the highest effectivity compared to other catalysts in zero-gap electrolysis. ECSA value of catalyst was comparable for all the prepared catalyst.

Acknowledgments

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EFFECT OF THE MEMBRANE AND CATALYST BINDER ON THE PERFORMANCE OF MEMBRANE-ELECTRODE ASSEMBLY IN ALKALINE WATER ELECTROLYSIS

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Hydrogen has been recognized as an integral part in decarbonization of the transport and industry. It can be used for: i) energy storage that contributes to renewable energy production stabilization, ii) as a fuel or iii) chemical feedstock. Water electrolysis is considered one of the most promising methods for producing hydrogen due to various advantages including to possibility of using renewable energy, no greenhouse gas emission, and high efficiency.

Alkaline water electrolysis (AWE) utilizes non-noble-metal catalysts and has been established as large-scale industrial technology. For the adaptation of AWE toward renewable energy sources utilization, further improvement of safety, flexibility and operation range is essential. Current AWE operates with 30 wt.% KOH solution due to separation of the electrode chambers by a thick, porous diaphragm. Due to intensive research, diaphragm can now be replaced by dense anion-exchange membrane, which allows the decrease of KOH concentration. Using membrane, catalysts can be deposited directly on the surface of the membrane (CCM). This approach improves the utilization of the catalyst and thus enables the catalyst loading reduction. Problem here represents the limited availability of appropriate polymer materials and lack of the knowledge on CCM systems.

The aim of this work is to verify the influence of different anion-exchange materials on the CCM performance. Here, block copolymer functionalized by 1,4-diazabicyclo[2.2.2]octane and Fumapem® membranes are used as membranes and catalyst binders. Non-platinum catalysts are deposited directly on the surface of the membrane. The obtained results show the possibility of performance and stability improvement by using suitable membrane and binder material.

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2D AND 3D MATHEMATICAL MODEL OF THE ALKALINE FUEL CELL STACK – DESIGN OPTIMIZATION AND PARASITIC CURRENT ANALYSIS

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Alkaline hydrogen fuel cells (AFC), nowadays, represent a promising alternative fuel cell technology enabling direct conversion of the chemical energy bound in the hydrogen molecule to electric energy. AFCs have many advantages as compared to the most widespread hydrogen PEM-type fuel cells. The alkali environment allows the usage of non-platinum group catalysts and fast kinetic of the oxygen reduction reaction. However, the AFCs have to be carefully designed with respect to the value of parasitic (bypass, shunt) currents responsible for notable current efficiency losses.

The present work is focused on the development of mathematical models enabling analysis of the parasitic current distribution and following engineering optimization of the AFC stack. A 2-dimensional (2D) and 3-dimensional (3D) model representing laboratory-size (single cell active area of 5x5 cm^2) AFC stack in the bipolar arrangement were developed, based on the model of secondary current density distribution. The 3D model describes the laboratory AFC stack with all geometrical details, thus brings an opportunity to realize precise calculation of current distribution, parasitic current value, power output and energy efficiency. This model was validated by the 4-cells laboratory AFC stack. However, the 3D model is highly demanding on the computer hardware performance and computing time, which is not feasible for larger stacks simulation. Due to this a simplified 2D model version was proposed and validated by the 3D one. The validated 2D model is then equally accurate as the 3D one and, moreover, is more suitable for engineering design and optimization of stack geometry with a higher number of cells and larger active area. From this modelling study results that the current AFC stack is optimized with respect to parasitic current. The predicted efficiency is around 99.5 % at the maximal power output of 12.8 W and output current value of 8 A in the 4-cells arrangement. With an increased number of cells, the efficiency slightly decreases. The chosen multiscale approach employing the benefits of both 3D and 2D model has been demonstrated as an effective engineering design and optimization tool.

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ALKALINE WATER ELECTROLYSIS FOR ENERGY CONVERSION – IMPACT OF THE SEPARATOR TYPE ON THE CELL OPERATIONAL CONDITIONS

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Alkaline water electrolysis represents the traditional way of hydrogen production. For more than century it, however, cannot compete economically with hydrogen production from fossil fuels. Nowadays the situation is changing, as the diversification of energy and raw materials sources, as well as reduction of carbon dioxide emissions come to the centre of interest. Water electrolysis represents one of the few technologies offering alternative way for produce raw materials with significantly reduced, or no carbon dioxide emissions. At the same time, hydrogen can serve as an energy vector and thus allow storing large amount of electrical energy in a form of the chemical one. This is why it is within the last two decades attracting more and more attention not only of the research community.

Despite traditional approach to the alkaline water electrolysis was based on utilisation of the concentrated KOH solution as an electrolyte, more recently so called PEM (Proton Exchange Membrane) seemed to offer more attractive option. It was mainly because of high process intensity and flexibility. Therefore, research activities focused primarily on this process. Despite all effort, however, this technology can still not operate without utilising high amount of precious metals as catalysts of the electrodes reactions. Therefore, researchers turn currently their attention to the development of and alkaline technology utilising, however, alkaline polymer electrolyte membrane as a solid electrolyte and electrodes compartments separator in one. This would, in an ideal case, mimic PEM process, however, without need of utilising precious metals based catalysts. Nevertheless, development of this innovative technology faces several important issues.

The topic of this contribution is to provide basic introduction to and comparison of the alkaline water technologies utilising KOH solution and alkaline polymer membrane as electrolytes. Special focus will be on the role of separator and its impact on operational conditions of the laboratory scale electrolysis cell.

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MODELLING HYDROGEN PRODUCTION FROM RENEWABLE SOURCES OF ENERGY USING ALKALINE WATER ELECTROLYSIS

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The inevitable shift towards green energy is posing various challenges on energy sector transformation and optimization. Most renewable sources of energy are not controllable; therefore, their production cannot be synchronized with the energy demand. The produced electricity needs to be stored in a way which allows long-term storage, easy transport and effective transformation back to electricity or to other forms of energy.

Hydrogen can serve as such energy carrier. It can be produced using green electricity by water electrolysis which results in a clean, ecological product. Hydrogen can be used in various fields of chemical industry or used to produce electricity in hydrogen fuel-cells as a stable source of electricity or in the transport sector. For example, hydrogen-powered trains are large consumers of hydrogen. Production and storage of H_2 can compensate difference between energy production and energy need.

Proper design of an electrolyser in relation to the properties of its intended power source has a direct impact on the utilization of the system and maximization of hydrogen production. A simple mathematical model was created to assess hydrogen production by classical alkaline water electrolysis used regularly in the industry and by novel membrane alkaline water electrolysis. The model offers to change the dimensions of the electrolyser, number of cells or standalone electrolyser units and variable operating conditions. Data for three photovoltaic power-plants from Czechia, Slovakia and Hungary was used as model profiles of photovoltaic power-production in a given area.

This model can be used as a valuable tool for electrolyser utilization optimization for maximal hydrogen production using renewable sources of energy.

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3D PRINTED FLOW CELL FOR THE ELECTROCHEMICAL DETERMINATION OF ANTIBIOTICS

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Recent years, the incomplete removal of antibiotics from wastewater by standard treatment methods has turned out to be a serious problem causing increased bacterial resistance in the aquatic environment. In the case of modern pharmaceuticals wastewater treatment plants (WWTPs) are often unable to ensure their complete mineralization. One of the micropollutants that passes through the WWTP almost untouched is ciprofloxacin (CIP), which is a broad-spectrum antibiotic that is widely used for the treatment of various kinds of infections. The massive use of this antibiotics and its inefficient removal leads to increased amounts of its residues in the aquatic environment causing bacterial resistance. Therefore, monitoring the concentration of these harmful substances directly in the effluent wastewater is essential. The fact that in the real sewage system, the determination of these micropollutants needs to be performed in the convective regime calls for the development of electrochemical techniques operating under flowing conditions. In this work we designed and manufactured a 3D printed flow cell simulating the flowing sewage system in WWTPs. We explored the capabilities of electrochemical determination of CIP by studying the effect of sample flow rate, analyte concentration and voltametric flow rate. Cyclic and square-wave voltametric study of CIP was performed employing boron-doped diamond screen-printed electrodes. The obtained results confirmed that due to convection the mass transport rate increases in the flow cell. The acquired Faradaic response was in scale with the sample flow rate according to the prediction given by Levich equation. The findings that we achieved through this work demonstrate the feasibility of electrochemical monitoring of micropollutants in the flowing wastewater systems.

This work was supported by the Slovak Research and Development Agency under the contract no. APVV-21-0076 and by Norway through the Norway Grants; project: “Innovative carbon-based sorbents as an effective method of wastewater treatment”, grant number 3213200008.

THE CHARACTERIZATION OF INORGANIC NANOMATERIALS USING ADSORPTION TECHNIQUE

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A Inorganic nanomaterial means a natural, incidental or manufactured material containing particles as aggregates, agglomerates or particles in unbound state, where 50% or more of them range in the number of size distribution and one or more external dimensions are in the size range of 1 nm-100 nm. (One of the possible definitions of the nanomaterials). Where technically feasible and requested in specific legislation, the compliance with the definition may be determined on the basis of the specific surface area by volume (VVSA). A material can be considered falling with the definition, when the volume specific surface area of material is greater than 60 m^2/cm^3. However, the material, which according to its size distribution value belongs to nanomaterials, can be considered complying with the definition even if its specific surface area is lower than 60 m^2/cm^3 [1].

The volume-specific surface area of a particulate material is one of two apparently very different metrics recommended by the European Commission for the definition of nanomaterial. The volume-specific surface area is property of materials, which is obtained by dividing the samples external surface (S) by its solid volume (V) or by multiplying the specific surface area (SSA) by the materials skeletal density (ρ). It is conventionally stated in units of m^2/cm^3 and its value depends on the particle size and size distribution: small particles have a large volume-specific surface area and vice versa. For dry powders, the volume-specific surface area can be determined via the gas-adsorption measurement of the specific surface area by nitrogen (with adsorption isotherms of type II, III or IV according to the IUPAC classification), and multiplying it by skeletal density from the He-pycnometry measurement. In this study was evaluated the potential of the volume-specific surface area method as a classification tool, both for the identification of nanomaterials and of non-nanomaterials. For nonporous materials: When deriving the average size of the smallest particle dimension from volume-specific surface area, taking into account the approximate particle shape (sphere, fiber, plates) is a good agreement with the electron microscopy results. Achieving such a good agreement is also possible for porous particles using the t-plot method (not BET method), which is capable of separating the pore surface from the particles external surface.

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BIOTECHNOLOGY AND BIOREFINERY

THE ANNOTATION AND FUNCTIONAL DESRIPTION OF NON-MODEL BACTERIA FOR BIO-BASED ENGINEERING AND INDUSTRY

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The annotation and functional description of non-model bacteria requires new bioinformatics and systems biology tools for a comprehensive description of little studied microorganisms and inference of biological knowledge further utilizable in synthetic biology for engineering of industrially utilizable bacterial strains. Bacteria form the largest group of organisms in the world. Since the DNA and RNA sequencing became widely available, they begun to be often studied on molecular level for their exceptional biological properties, e.g., ability to produce fuels or plastics from waste. Unfortunately, previous lack of interest in their research is the source of many obstacles in bioinformatics and systems biology data processing as current tools, designed primarily for eukaryotic model organisms, cannot be easily used for processing data gathered from non-model bacteria. Inference of biological knowledge presumes identification of regulated genes and annotation of their molecular function so involved biological processes could be captured. This talk addresses two important questions, how to assemble a comprehensive functional annotation for non-model organisms and how it affects inferred biological knowledge. This can be achieved by designing novel pipelines utilizing high throughput sequencing data while considering data bias, and their combination with annotation build by extensive database searching. Eventually, the successful functional annotation can not only substantially contribute to our understanding of various microorganisms, but can show how various parameters of bioinformatics data processing affect resulting biological knowledge and provide ready-to-use solution for wide scientific community.

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ROD ANEURINIBACILLUS – UNIKÁTNÍ BAKTERIE MEZI TERMOFILNÍMI PRODUCENTY POLYHYDROXYALKANOÁTŮ

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Novou generací biotechnologického průmyslu jsou extremofilní organismy. Tyto organismy dokážou žít a prosperovat pro nás v nehostinných podmínkách jako jsou vysoká či velmi nízká teplota či velké extrémy pH prostředí, vysoké koncentrace soli nebo těžkých kovů. Využití těchto organismů přináší mnoho výhod do biotechnologického průmyslu. Navíc se mezi extremofilními organismy přirozeně vyskytují také bakterie, které jsou schopny produkovat polyhydroxyalkanoáty (PHA). PHA jsou mikrobiální polyestery, které jsou svými vlastnostmi podobné petrochemickým polymerům a jsou jejich vhodnou alternativou. PHA jsou také plně biodegradabilní a biokompatibilní, což přináší jednak ekologickou úlevu, ale také široké spektrum použití těchto materiálů. Navíc lze jako zdroj uhlíku pro bakterie využít nějaký odpadní substrát čím dochází ke snížení provozních nákladů a tím i ke snížení ceny výrobku.

V rámci naší experimentální práce jsme se zaměřili na izolaci nových termofilních producentů PHA a zhodnocení jejich biotechnologického potenciálu. Pomocí originálního izolačního protokolu bylo izolováno několik zástupců rodu *Aneurinibacillus*. Aneurinibacilli se ukázaly jako zajímaví producenti PHA s velkým potenciálem. Tyto bakterie jsou schopny produkce nejen homopolymeru složených pouze z jednotek 3-hydroxybutyrátu (3HB) ale i kopolymerů, které kromě monomeru 3HB obsahují i 4-hydroxybutyrát nebo další velmi neobvyklé monomery jako jsou 3-hydroxyvalerát, 4-hydroxyvalerát nebo 5-hydroxyvalerát. Také jejich metabolismus syntézy PHA je odlišný od běžných producentů PHA.

Kromě produkce PHA s unikátními monomery je tento rod také schopen produkce biosurfaktantů, kde jejich supernatant tvořil s hexanem emulzi, kdy byl emulgační index (E_{24} 57,4) srovnatelní s roztokem 5% Tritonu X-100. V rámci studia biotechnologického potenciálu bylo také zjištěno, že je tento rod schopen produkovat celulázy, xylanázy či lipázy. V rámci studia tohoto zajímavého rodu byly také sestaveny kompletní genomy vybraných kmenů.

V současné době se soustředíme se na kultivac těchto mikroorganismůi v bioreaktorech, kdy koncentrace biomasy dosahuje až 6,3 g/l a produkce PHA dosahuje téměř 2 g/l se zastoupením přes 70 mol. % 4HB v kopolymeru.

VYUŽITELNOST TERMOFILNÍCH BAKTERIÍ JAKO PRODUCENTŮ BIOPOLYMERŮ

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Termofilní bakterie jsou podskupinou extremofilních mikroorganismů. Tyto bakterie prospívají v prostředí s vyššími teplotami, které jsou pro ostatní mikroorganismy leckdy letální. Termofilní bakterie jsou důležité pro průmyslové účely především pro produkci enzymů, ale například i pro výrobu biopaliv. Jejich termofilní charakter představuje mnoho výhod. Jedním z nich jsou nižší nároky na sterilitu prostředí, jelikož je výrazně eliminováno riziko mezofilní kontaminace, která se v průmyslu poměrně běžně vyskytuje. Dalšími bonusy jsou nižší spotřeba vody pro chlazení celého procesu či vyšší rozpustnost některých substrátů. Potenciál termofilů představuje také produkce polyhydroxyalkanoátů (PHA).

PHA jsou biodegradabilní a biokompatibilní biopolymery. Svými vlastnostmi mohou nahradit některé komerční plasty, které způsobují globální environmentální problémy. PHA polymery mají mnoho výhod, nicméně jejich produkční cena je stále vyšší než u plastů vyráběných z ropy. Tyto náklady mohou být sníženy právě použitím termofilních bakterií. Z tohoto důvodu byl proveden základní screening biotechnologického potenciálu u vybraných termofilních bakteriálních rodů, z kterých byly následně vybráni slibní zástupci. Z mnoha kandidátů se jako nejlepší kmeny jeví bakterie *Schlegelella thermodepolymerans* DSM 15344^T a *Tepidimonas taiwanensis* LMG 22826^T. Obě bakterie jsou schopny výrazného nárůstu biomasy a současné akumulace PHA. *S. thermodepolymerans* je unikátní ve své schopnosti utilizovat xylózu výrazně lépe než jakékoliv jiné substráty. *T. taiwanensis* je kromě produkce PHA také zdrojem termostabilních proteáz. V souladu s konceptem průmyslových biotechnologií nové generace (Next Generation Industrial Biotechnology) je také testována schopnost produkce PHA z odpadních substrátů, díky čemuž je taktéž možné snížit celkové produkční náklady těchto biopolymerů.

ROBOLECTOR XL® – FUTURE OF OPTIMIZATION AND AUTOMATIZATION OF MICROFERMENTATIVE PROCESSES FOR ACCELERATED SCALE-UP AND STREAMLINED RESEARCH APPLICATIONS

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Optimization and scale-up of bioprocess is important step from fundamental research to industrial practice and can be very time-consuming, expensive, and quite challenging – usually calling for multidisciplinary team of biotechnologists, microbiologists and engineers. The scale-up starts in laboratory measure in microtiter plates or flasks and follows across laboratory bioreactor up to half-operation or industrial bioreactor. Such process can turn very difficult and asks for complex modelling and possible prediction of extreme states, which could otherwise destroy the instrumentation in the process when tested experimentaly[1]. M2P Labs came up with an elegant solution to ease such process more than decade ago.

Biolector (Robolector when merged with robotic instrument assisting measurement and preparation of media/solutions) is an elaborate microcultivation device providing an opportunity to online-observe biomass content, pH value, DO_2/DCO_2 or fluorescence of 36-48 samples in range of temperature 5-50 °C all during ongoing cultivation. All measurements take place during the cultivation without a need for stopping the shaking of the batch by light scatter scanning at the bottom of each well in plate. In addition, the device could use special microfluidic plates, which enable nutrient/inductor feeding and pH controlling during the process thus mimicking the bioreactor in smaller volumes. Such management of microcultivations provide similar outcome as the lengthy optimization process as mentioned above. Numerous studies compared Biolector and routine bioreactors or cultivations in flasks and found great reproducibility of Biolector results in greater volumes[2,3]. Biolector XT is suitable for bacterial and yeast cultivations, it can be used also for anaerobic processes[4] or even cultivation of filamentous microorganisms[2].

For possible cooperation please contact the corresponding author or see:
https://www.m2plabs.com/bioreactors/robolector/robolector-xl/.

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CHARACTERIZATION OF PROBIOTIC BACTERIUM *CLOSTRIDIUM BUTYRICUM*

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Clostridium butyricum strain CBM 588 is approved in the EU for human consumption as a so-called novel food ingredient that can be used in human food supplements and also as an additive for animals, such as chickens. The bacterium is strictly anaerobic, rod shaped and spore-forming. The main products of its metabolism include lactic, butyric and acetic acids, carbon dioxide and hydrogen. The probiotic effect of this bacterium is associated with the formation of spores and their germination in the large colon. It is easier for the spores to pass through the gastrointestinal tract and resist the action of stomach acid, bile salts and colon enzymes than for the vegetative cells of most other probiotics. Although this strain was isolated as early as 1933, it has been relatively little studied. Therefore, different culture conditions, inoculation methods and management of the culture process have been tested to facilitate spore formation and/or acid production, especially butyric acid. It is likely that the main factors leading to the initiation of the sporulation cascade are a suitable pH, an excess of carbohydrates in the culture medium and the attainment of a certain population density.

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INNOVATIVE APPROACHES FOR REUSING ANIMAL BY-PRODUCTS

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Waste valorisation, which emphasises reusing and recycling waste products, is gaining prominence due to the circular economy approach. The poultry sector is the fastest-growing meat market, with global consumption projected to reach 153.85 metric kilotons by 2031 (1). But, this increased production also creates a significant increase in waste, which can be reused to fulfil the circular economy concept and make the industry more efficient and profitable.

One low-value by-product, formed after mechanical meat separation (W-MSM), is rich in cartilage, bones, skin, muscle and adipose tissue. W-MSM can be further processed concerning the different final usage, for example: i) can serve as a source of bioactive compounds (product HyaTide) such as hyaluronic acid, chondroitin sulphate, peptides and amino acids (2); ii) can be used in stimulation therapy because the fraction of HyaTide was proved to have immunostimulating activity; or iii) after the pyrolysis can be used as biochar in agriculture (3), where can significantly improve the soil properties and supplement the source of phosphorus (P). This is very important due to the no geological deposit of P in Europe and predicted P shortage and depletion.

In addition, the poultry industry generates around 5 million tons of chicken feathers annually, and due to restrictions or bans on classical disposal methods, there is a growing demand for environmentally friendly technologies for processing feather waste. We proved that feathers could be converted into hydrolysate rich in soluble peptides and amino acids and, therefore, can be used as a low-cost cultivation medium for the growth of microorganisms (4). Within this new project, we will implement the wastes from the poultry industry as replacement nutrient media for bacteria capable of microbiological calcite precipitation (MICP) technology to form a composite sample called bio-concrete from a fine fraction of construction and demolition wastes.

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THE POTENTIAL OF *MONASCUS* SPP EXTRACTS AS PHOTOSENSITIZERS IN ANTIMICROBIAL PHOTODYNAMIC THERAPY

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The antimicrobial resistance and the increasing number of multi-drug resistant bacteria are a global public health threat. The promising way of bacterial infection treatment is antimicrobial photodynamic therapy (aPDT). In aPDT a light source is used independently or with the presence of photosensitizers. In this study, we tested the potential of fungus *Monascus* secondary metabolites as the photosensitizers. The extracts were prepared from red yeast rice and mycelia of *Monascus purpureus* DBM 4360 and *Monascus* sp. DBM 4361. The effects of extracts on model microorganisms were evaluated after exposure to dark conditions or blue light irradiation. All of the *Monascus* extracts showed antimicrobial activity against gram positive bacteria with a higher toxicity measured after irradiation. The antimicrobial activity against gram negative bacteria was observed only after irradiation. Yeast was not susceptible in dark nor after irradiation. The differences between extracts from the two strains were observed. However, the overall trends were similar. Our results indicate, that the fungus *Monascus* is a promising source of photosensitizers.

EVALUATION OF PACKAGING MATERIALS FOR BIOFILTERS: PREDICTION AND VERIFICATION OF BIOFILM DEVELOPEMENT

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The packaging material in biofilters plays a key role as a biofilm carrier. Detailed studies of their surface properties and ability to serve as a biofilm carrier are scarce. Therefore, the aim of this work was to perform experiments aimed at characterizing 7 packaging materials with potential use as part of the mixed packaging material of biofilters. The selection of the most suitable material(s) was made based on its cost, physicochemical properties and operational parameters, etc. surface properties and biofilm formation kinetics, bulk density, and porosity.

The first part of the study was to predict the development of biofilm formed by *Pseudomonas* sp. on the selected materials. It was necessary to determine the physicochemical properties of the materials and cell surface. Therefore, the contact angle and zeta potential were determined. These values are the basis for the thermodynamic model and XDLVO theory that predict cell-surface interaction. The second part was focused on the experimental determination of biofilm formation. An experimental biofilm reactor was used to measure its kinetics. Finally, the operational properties of the packages were determined.

Significant differences in the surface properties of the materials and cell were found. The order of hydrophobicity was as follows: *Pseudomonas* sp. > oak > spruce > root > sludgechar > biochar > Liapor > vermiculite. While the order of zeta potential was as follows: *Pseudomonas* sp. > biochar > sludgechar > vermiculite. Thus, *Pseudomonas* cells was rather hydrophobic especially in comparison with surface of materials and with less zeta potential that materials. Experimental determination of biofilm formation showed the following order of biofilm coverage after 4 h: biochar > sludgechar > vermiculite > Liapor > oak > spruce > root. This 4-hour time interval corresponded to primary adhesion and was only partially consistent with predictions.

STŘÍBRNÉ NANOČÁSTICE PŘIPRAVENÉ S VYUŽITÍM VINOHRADNICKÉHO ODPADU -CHARAKTERIZACE A BIOLOGICKÁ AKTIVITA

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Stříbrné nanočástice jsou dobře známé svými pozoruhodnými fyzikálními, chemickými a biologickými vlastnostmi. V mnoha oblastech, jako je medicína nebo textilní a potravinářský průmysl, najdeme nanočástice stříbra jako antimikrobiální činidla. Konkrétně se se stříbrem v podobě nanočástic můžeme setkat v obvazech na popáleniny, textilu nebo některých dezinfekčních prostředcích. Nanočástice stříbra lze připravit třemi základními způsoby – fyzikálními, chemickými nebo biologickými metodami. S tím, jak roste poptávka po produktech obsahující nanostříbro, snažíme se hledat způsoby jeho výroby, které by byly nenákladné, jednoduché a navíc šetrné k životnímu prostředí. Atraktivní je syntéza nanočástic metodami biologickými, jež k redukci iontového stříbra a zároveň i stabilizaci vznikající nanočástice využívají biologické materiály. Pozornost si jednoznačně zaslouží především syntéza nanočástic pomocí rostlinných extraktů připravených s využitím odpadních produktů zemědělské nebo potravinářské výroby (např. slupky nebo skořápky).

Tato práce je zaměřena na využití vinohradnického odpadu k syntéze stříbrných nanočástic o různé velikosti, jejich charakterizaci a testování antimikrobiálních účinků. Nanočástice stříbra byly připraveny pomocí ethanolového extraktu drcených letorostů *Vitis vinifera* a byly charakterizovány analytickými technikami jako je UV-vis spektroskopie, skenovací elektronová mikroskopie ve spojení s energiově disperzní spektrometrií a infračervená spektroskopie s Fourierovou transformací. Antimikrobiální aktivita připravených nanočástic byla sledována vůči podmíněně patogenním bakteriím (*Escherichia coli*, *Pseudomonas aeruginosa* a *Staphylococcus aureus*) a kvasinkám (*Candida* sp.). Vliv nanočástic (0–80 mg/l) na růst suspenzních buněk byl sledován pomocí měření optické denzity rostoucí kultury v čase. Navíc byla použitím resazurinové eseje a metody MTT sledována schopnost nanočástic (0–20 mg/l) bránit tvorbě biofilmu zmíněných patogenů. Antimikrobiální účinky byly ve zkoumaném koncentračním rozmezí prokázány vůči suspenzním buňkám Gram negativních (G-) bakterií i kvasinek, naopak růst G+ zástupce *S. aureus* se nepodařilo v porovnání s kontrolou významně snížit. Podobně i inhibice tvorby biofilmu byla zaznamenána pouze u G- bakterií a kvasinek rodu *Candida*.

ANTIMICROBIAL ACTIVITY OF LIGNIN-BASED NANOSYSTEMS

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The key to the economic viability of a lignocellulosic biorefinery is the efficient conversion of all three major components of lignocellulosic biomass into value-added products. In this regard, the use of lignin is considerably limited due to its complex structure. One of the currently considered options for the use of lignin is its transformation into nanoparticles, in which the material shows different physicochemical properties, which allows expanding the use of this polymer to other fields of application. However, the properties of the resulting nanoparticles depend on the quality of the lignin itself, which is conditioned by the choice of the lignocellulosic biomass pretreatment method. A promising method, is the organosolv process, which delivers a high purity lignin with good solubility in organic solvents. In this work, lignin extracted from beech wood sawdust by organosolv fractionation at 180 °C for 60 min in a 60% v/v ethanol to water solution containing 1% w/w H_2SO_4 per dry weight of solids, was used to prepare nanoparticles. We developed synthesis procedures for the preparation of lignin nanoparticles that form stable colloidal dispersions in aqueous solutions; such colloidal dispersion is usually impossible to achieve with raw lignin. The presumed antimicrobial effects of lignin-based nanosystems, including damage to the bacterial cell wall due to the presence of polyphenols in the lignin structure and possible disruption of homeostasis after penetration into the bacterial cell due to the nanoscale, were subsequently tested.

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TERMÁLNÍ RADONOVÉ PRAMENY JAKO ZDROJ EXTRÉMOFILNÍCH MIKROORGANISMŮ

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Extrémofilní mikroorganismy se vyskytující v různých nehostinných prostředích po celém světě. Horké prameny, ledovce a hydrotermální průduchy jsou jen některé příklady extrémních prostředí, na která se extrémofilové adaptovaly. K překonání nepříznivých podmínek disponují tyto mikroorganismy mechanismy, které chrání biomolekuly před oxidačním stresem. Lze je rozdělit na antioxidační enzymy a neenzymatické systémy zahrnující karotenoidy, manganaté kationty a extracelulární polymerní látky. Dále tyto mikroorganismy často disponují účinnými mechanismy opravy DNA.

Mikroorganismy odolné vůči ionizujícímu záření nebo oxidačnímu stresu se vyskytují v rozmanitých habitatech jako vysokohorská jezera, pouštní půdy nebo prostředí přirozeně či antropogenně zatížené radionuklidy. Na území České republiky lze očekávat výskyt takovýchto mikroorganismů například v bývalém stříbro-uranovém dole Svornost v Jáchymově (Joachimstahl). Dnes se jedná o nejhlubší důl sloužící k těžbě vody, která je v důsledku rozpadu radia v jáchymovském podloží nasycena radonem (^{222}Rn ~ 24 kBq/l) a využívá se pro své léčebné účinky. Vzhledem k zvýšené přítomnosti přírodních radionuklidů lze tuto lokalitu považovat za nehostinné místo pro jakoukoli formu života. Na základě výsledků z již provedených rozsáhlých mikrobiálních analýz podobných lokalit lze předpokládat, že i v dole Svornost se mohou vyskytovat různé radiotolerantní nebo radiorezistentní mikrobiální komunity zajímavé jak z taxonomického a/nebo biotechnologického hlediska.

Tato práce je věnována izolaci a charakterizaci bakterií ze 4 pramenů z Jáchymova (C1, Curie, Běhounek a Agricola). Z desítek izolátů bylo na základě screeningu vybráno celkem 6 nejodolnějších izolátů, které byly dále podrobeny testům resistence. Vzhledem k nepřetržité expozici mikroorganismů ionizujícímu α-záření z jáchymovských radioaktivních pramenů, které způsobuje intracelulární tvorbu reaktivních forem kyslíku (ROS), lze u izolátů získaných z těchto pramenů předpokládat zvýšenou toleranci/odolnost vůči oxidativnímu stresu. Na základě tohoto předpokladu byla provedená sada testů, při kterých byly jako intracelulární induktory ROS použity mitomycin
a peroxid vodíku. Dále byla provedená analýza odolnosti vůči UV a gama záření.

EPOXIDATION OF ESTERS FROM VEGETABLE OILS – REACTION CONDITIONS AND STATISTICAL EVALUATION

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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 rapeseed and linseed oil was carried out with performic acid. The influence of reaction conditions (such as time, temperature, molar ratios between reactants, etc.) on properties of epoxides (such as iodine and epoxide value, relative conversion to oxirane, kinematic viscosity, etc.) was studied. The mutual relations between them were statistically evaluated and mathematical models were constructed. Generally, higher (i) initial iodine value of esters, (ii) reaction temperature, (iii) concentration of formic acid and longer reaction time caused more formed epoxides. On the contrary, higher concentration of hydrogen peroxide caused the epoxide ring opening and so formation of side products. The catalyst (H_2SO_4) and the intensity of stirring were statistically insignificant. Moreover, the drying of epoxides was carried out by distillation, which was significantly improved by the addition of small amount of methanol. The formed models (verified by independent experiments) allow to synthesize epoxides, which are biodegradable, non-toxic and have a variety of applications, such as biolubricants, biofuel additives, precursors for chemicals or CO_2 capture function.

Acknowledgements
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OTOČNÝ FOTOBIOREAKTOR PRO KULTIVACI SNĚŽNÝCH MIKROŘAS V EXTRÉMNÍCH KLIMATICKÝCH PODMÍNKÁCH

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V polárních oblastech byly izolovány kmeny sněžných mikrořas, které jsou bohaté na cenné látky, např. nasycené mastné kyseliny, antioxidanty, karotenoidy nebo fenolické sloučeniny a další bioaktivní látky. Vedle produkce doplňků stravy nebo krmiv mohou být kultivační systémy využity v konceptech biorafinérií nebo pro čištění odpadních vod. Sněžné mikrořasy, na rozdíl od konvenčních sladkovodních mikrořas jako je např. Chlorella, jsou schopny růst při nízkých teplotách blížících se bodu mrazu a při nízkých intenzitách slunečního záření. Adaptace sněžných mikrořas klimatickým podmínkám střední Evropy, konkrétně České republiky, by mohla prodloužit celkovou dobu kultivace v průběhu roku a dále tak přiblížit kultivaci mikrořas komerčnímu průmyslovému využití. Pro zajištění efektivní kultivace mikrořas je klíčovým faktorem dostatečná intenzita světelného záření, která na principu fotosyntézy umožňuje růst mikrořasové biomasy. Pro účely kultivace sněžných mikrořas byl navržen otočný deskový fotobioreaktor, který je schopen využívat maximální potenciál nepřetržitého slunečního svitu v průběhu polárního dne. Na základě místa instalace fotobioreaktoru a aktuálního času v dané lokalitě řídící systém otáčí desku fotobioreaktoru podle aktuální polohy slunce. Paprsky slunečního záření tak dopadají vždy kolmo na transparentní plochy komory deskového fotobioreaktoru, čímž dochází k maximálnímu využití fotosynteticky aktivního záření k růstu buněk mikrořas. Konstrukce fotobioreaktoru musí být zároveň uzpůsobena tak, aby odolávala nízkým teplotám, vysoké vlhkosti a prašnosti okolního prostředí. První dlouhodobá kultivační kampaň prokázala vhodnost použití navržené konstrukce fotobioreaktoru. Navržená koncepce otočného fotobioreaktoru může být dále použita pro kultivaci mikrořas v zimních měsících v České republice. Na základě ověřeného prototypu bude vytvořena metodologie zvětšování měřítka do průmyslového měřítka.

MICROALGAE DISINTEGRATION USING A LABORATORY BEAD MILL

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Disruption of the microalgal cell wall is one of the key processes in the concept of microalgal biorefinery, mainly due to the desired extraction of valuable chemicals which are stored inside the cells [1]. One of the common methods of cell wall disruption is the bead milling, a method mainly used due to its high cell disruption rate and general reliability [2]. However, its high energy consumption makes it less favourable for industrial application. This drawback may be overcome through understanding of the underlying process and its optimalization [3]. To explore the amount of energy required to achieve cell disruption a laboratory bead mill was designed which utilizes agitator batch mixing (Figure 2.). The main benefits of the novel laboratory mill are the uniform distribution of power input throughout the batch, small and easily defined area in which high energy impacts occur and easy power input measurement. In this study, basic characteristics of the mill are explored with the assessment of its functionality.

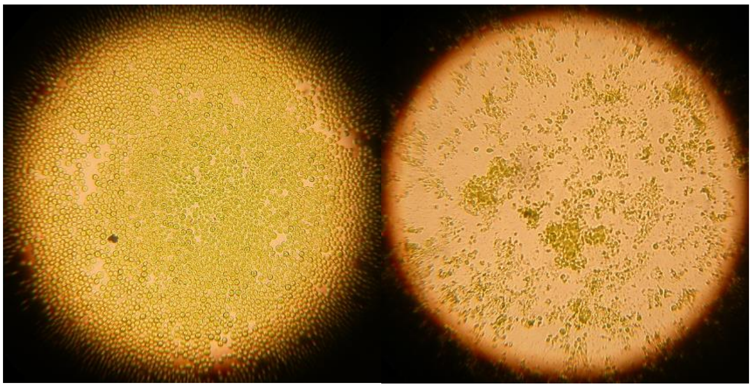

Figure 1. Comparison of cell structure
before and after milling

Figure 2. Photo of the laboratory mill

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PRODUKCE UNIKÁTNÍCH PHA KOPOLYMERŮ TERMOFILNÍMI GRAMPOZITIVNÍMI BAKTERIEMI RODU *ANEURINIBACILLUS*

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Znečištění životního prostředí syntetickými plasty, které jsou často získávány z ropných zdrojů, je jedním ze stále narůstajících problémů dnešní doby. Jistou formu úlevy nabízí využití mikrobiálních polymerů, tzv. polyhydroxyalkanoátů (PHA). Díky jejich mimořádným vlastnostem, mezi které patří především biodegradabilita, biokompatibilita a netoxicita, nabízí PHA materiály vhodnou alternativu k syntetickým plastům v mnoha aplikacích (lékařství, spotřební a potravinářský průmysl atp.).

Nejhojněji produkovaným PHA polymerem je poly(3-hydroxybutyrát) (poly(3HB)), který však nemá v porovnání s klasickými plasty zcela ideální vlastnosti – vyznačuje se poměrně vysokou krystalinitou, která ho činí tuhým a křehkým. Řešení nabízí začlenění různých PHA monomerů do celkové struktury biopolymeru. To má za následek snížení krystalinity materiálu a zvýšení celkové elasticity, díky čemuž se PHA materiál svými vlastnostmi přibližuje běžným ropným plastům. Termofilní grampozitivní bakterie rodu *Aneurinibacillus* byly již dříve popsány jako producenti kopolymeru, který kromě 3-hydroxybutyrátu obsahoval také 4-hydroxybutyrát. Cílem této studie bylo hlubší prozkoumání diverzity syntézy PHA těmito bakteriemi.

Bakterie rodu *Aneurinibacillus* prokázaly produkci netypických PHA monomerů, jako je 4-hydroxyvalerát (produkce až do 69,3 mol.% z celkového obsahu PHA), 4-hydroxyhexanoát (až 31,9 mol.%) a 5-hydroxyvalerát (až 47,1 mol.%) a to pomocí laktonů (v kombinaci s glycerolem, koncentrace 4+4 g/l), které sloužily jako specifické PHA prekurzory. Dále bylo zjištěno, že získané PHA materiály jsou oproti homopolymeru poly(3HB) více amorfní a mohou tak vykazovat lepší mechanické vlastnosti. Využití termofilních bakterií navíc přináší do produkce PHA jisté úlevy v nákladech spojených s čistotou a sterilitou prostředí. Bakterie rodu *Aneurinibacillus* se tak jeví jako unikátní PHA producenti a jejich potenciál bude nadále zkoumán.

BIOTRANSFORMACE FERULOVÉ KYSELINY POMOCÍ EXTREMOFILNÍCH BAKTERIÍ

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Ferulová kyselina je fenolická sloučenina, která se běžně vyskytuje v buněčných stěnách rostlin. Je součástí lignocelulózových materiálů, které představují odpadní materiál vznikající v potravinářském průmyslu. V lignocelulóze je ferulová kyselina kovalentně navázaná na hemicelulózy a lignin. Pomocí izolačních postupů je možné ferulovou kyselinu z těchto materiálů uvolnit a využít na biotransformační experimenty.

Biotransformací se rozumí metabolická přeměna sloučenin pomocí živých organismů. Biotransformace ferulové kyseliny na látky s přidanou hodnotou, jako jsou vanilová kyselina, vanilylalkohol, vanilin či 4-vinylguajakol, je realizována pomocí mikroorganismů. V této práci byly využity extremofilní bakterie. Tyto bakterie jsou schopny přežívat v prostředí s extrémními podmínkami, které se vyznačují např. vysokou/nízkou teplotou, kyselým či zásaditým prostředím, nebo vysokou koncentrací solí. Díky jejich schopnosti přežívat v podmínkách, jež jsou pro ostatní mikroorganismy nepříznivé, je sníženo riziko kontaminace a tím pádem i náklady na výrobu požadovaných látek.

Zaměřili jsme se na konverzi ferulové kyseliny na vanilovou kyselinu pomocí extremofilních bakterií, konkrétně termofilních a halofilních kmenů. Vanilová kyselina nachází uplatnění v kosmetice či farmacii. Vykazuje neuroprotektivní účinky, díky čemuž ji lze využít k prevenci neurologických onemocnění (Parkinson, Alzheimer, roztroušená skleróza). Experiment byl realizován v baňkách, kdy byla ke kultivačnímu médiu (komplexní/produkční) přidána ferulová kyselina o různých koncentracích. Při kultivaci v produkčním médiu docházelo nejen ke konverzi ferulové kyseliny, ale i k produkci polyhydroxyalkanoátů (PHA). PHA jsou polyestery, které jsou akumulovány mikroorganismy ve formě intracelulárních granulí a mají podobné vlastnosti jako syntetické plasty. Biotransformačními experimenty bylo dosaženo úspěšnosti konverze ferulové kyseliny na vanilovou z 80–90 %.

APPLICATION OF ANIMAL WASTE HYDROLYSATES AS HEAVY METAL REMOVER FROM BROWNFIELDS

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Due to their high content of amino acids, fatty acids and/or proteins, hydrolysates from animal production waste are currently used, for example, as fertilizers to support the growth of the root system, protect plants, especially the leaf part, from excessive sunlight or to reduce water evaporation. They were also tested for protection of plants from pest attacks or browsing. They are also used as additives in pet food, increasing nutritional value.
Currently, great emphasis is placed on biologically acceptable procedures for the disposal of environmental burdens, such as the removal of toxic metals from soil or sewage sludge. The chelating effects of hydrolysates have already been proven in tests on soils from an industrial brownfield, containing heavy metals (As, Cd, Cr, Mn, Ni, Pb, etc.) of a former metallurgical plant.
The degradable hydrolysate, in addition to washing out metals, significantly supports the bio-stimulation of soil spore-forming bacteria by several orders of magnitude compared to other used chelating agents, such as EDTA (Chelaton II). Hydrolysate application promotes the growth of surfactant-producing microorganisms and could therefore be a possible inexpensive way to enrich the soil with desirable microorganisms. The hydrolysate thus represents a new ecologically acceptable chelating agent that can be used simultaneously as a fertilizer supplement.

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VÝVOJ TECHNIKY EKOLOGICKÉ IZOLACE POLYHYDROXYALKANOÁTŮ Z VYBRANÝCH EXTRÉMOFILNÍCH BAKTERIÍ

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Polyhydroxyalkanoáty (PHA) představují biodegradabilní alternativu k tradičním petrochemickým plastům. Zatímco lidé využívají výhodných mechanických vlastností těchto materiálů, mikroorganismy schopné jejich akumulace mají zvýšenou robusnost a tím i odolnost vůči řadě stresorů. Produkce PHA může proto představovat jeden z adaptivních mechanismů extrémofilů na jejich přirozené prostředí.

Pro experimenty byly vybrány dva extrémofilní kmeny, a to halofilní bakterie *Halomonas halophila* (CCM 3662) a termofilní *Schlegelella thermodepolymerans* (DSM 15344). Biotechnologická výroba PHA s využitím extremofilů v rámci konceptu průmyslové biotechnologie nové generace (NGIB) přináší do celého procesu řadu výhod s ohledem na požadavky na sterilitu, kultivaci a také specifické možnosti procesu izolace PHA.

Kombinace hypotonického šoku, zvýšené teploty oproti optimu pro vybrané kmeny a detergentu SDS po optimalizaci jednotlivých parametrů izolačního procesu vedly u obou etrémofilních producentů k zisku PHB s čistotou vyšší než 90 hm. %.

Unikátní vlastnosti vybraných extrémofilů lze tedy efektivně využít při ekologické a zároveň ekonomicky proveditelné izolaci PHA vysoké čistoty s možností následné recyklace zbytkového SDS.

ANTIMICROBIAL ACTIVITY OF RED PIGMENTS PRODUCED BY THE FUNGUS *MONASCUS*

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The genus *Monascus* includes representatives of filamentous fungi that has been commonly used in Asian countries in the food industry as a colouring agent or preservative for several hundred years. The fungus *Monascus* can produce bioactive metabolites, among which are substances belonging to the statins, monacolins. In addition, they can produce the mycotoxin citrinin. However, a characteristic feature of the *Monascus* fungus is the production of polyketide pigments, which give the fungus its characteristic red colour. The *Monascus* pigments can be distinguished according to their absorption maxima into yellow (390 nm), orange (470 nm) and red (500 nm). Red pigments are the most water-soluble pigments of all. In previous years, their anti-inflammatory and anti-obesity effect has been observed, as well as their antimicrobial effect against certain types of microorganisms. In our work, the effects of red pigments contained in the culture broth on the growth of yeasts, Gram-positive and Gram-negative bacteria was investigated. The highest effect of the red pigments was observed on the growth of Gram-positive bacteria *Lactobacillus plantarum, Lactobacillus acidophilus* and *Bacillus subtilis*, where the growth was significantly slowed, and the lag phase was prolonged. In the case of the Gram-negative bacteria *Escherichia coli* and *Pantoea agglomerans*, no effect of the pigments on growth was observed. When *Monascus* pigments were added to the yeasts *Saccharomyces cerevisiae, Zygosaccharomyces bailii* and *Candida utilis*, very low efficiency on their growth was observed.

VLIV TEPLOTY, SVĚTELNÉHO REŽIMU A SLOŽENÍ MÉDIA NA PRODUKCI PHA U CYANOBAKTERIÍ DRUHU *SYNECHOCYSTIS*

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Znečištění oxidem uhličitým je téma, které silně rezonuje společností. V roce 2021 bylo do atmosféry vypuštěno více než 35 miliard tun CO_2. Prostřednictvím přirozených cyklů Země se každý rok přirozeně absorbuje a vypustí 100 miliard tun oxidu uhličitého. Cyanobakterie neboli sinice jsou prokaryotické autotrofní organismy disponující oxygenní fotosyntézou. Sinice produkují širokou škálu pigmentů (chlorofyl, karotenoidy, fykocyanin), metabolitů s biologickou aktivitou antimikrobiální, antifugální, antiprotozoální, antimalarickou,... a dále zásobní látky jako glykogen, cyanophicin či polyhydroxyalkanoáty (PHA). PHA jsou mikrobiální biopolymery, které se v buňkách nachází v podobě intracelulárních granulí. PHA u sinic zaujímá primárně roli zásobních látek, kdy se vyskytují v podobě intracelulárních granulí. Fyzikálně-chemické vlastnosti PHA jsou podobné petrochemickým plastům, na rozdíl od nich jsou PHA biodegradabilní i biokompatibilní. Produkce PHA je nejen časově, ale i finančně náročná, pro snížení výrobních nákladů jsou jako vstupní suroviny využívány odpadní materiály- např. kávová sedlina, jablečné a vinné výlisky či mláto. Odpadní materiály slouží jako zdroj uhlíku a energie pro heterotrofní bakterie, jako je *Cupriavidus necator* H16 nebo *Halomonas halophila*. Jelikož jsou sinice schopny kyslíkové fotosyntézy, tak na rozdíl od heterotrofních bakterií sinice nevyžadují organický zdroj uhlíku. Pro syntézu PHA vyžadují pouze CO_2 a světlo. Technologie využívající odpadní CO_2 jako zdroj uhlíku pro sinice produkující PHA by mohla být velmi přínosná pro životní prostředí. Záchyt a následná fixace oxidu uhličitého spolu se snižováním emisí CO_2 za rok by mohlo zpomalit oteplování zemského povrchu. V této práci jsou představeny abiotické podmínky a jejich kombinace, které vedly k vyšším výnosům PHA v cyanobakteriální kultuře dvou zástupců rodu *Synechocystis*.

MODIFICATION OF MORPHOLOGY AND RHEOLOGICAL PROPERTIES OF BACTERIAL CELLULOSE BY PRODUCTION MEDIUM

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Bacterial cellulose is an extracellular polysaccharide produced by many bacterial strains as a protective envelope against the environment. It possesses unique mechanical and physical properties that enable a wide range of applications in medicine, cosmetics, electronics, textile and food industry or biotechnology. However, the main disadvantage of bacterial cellulose is its high production costs[1].

Food- and agricultural-based industries produce a vast quantity of waste with high sugar content or hemicellulose/cellulose that may be transformed into a carbon source for bacterial cultivation. About one third of all food produced globally is wasted annually[2]. This work is focused on the utilization of carbon sources present in grape pomace, banana peels or by-products arising during the isolation of lignin. The carbon sources were derived via hydrolysis of the waste mentioned above and the hydrolysates were used directly in media to cultivate *Komagataeibacter xylinus*. The tested hydrolysates have been proven to be suitable carbon sources for cultivating *K. xylinus*. The yields of bacterial cellulose produced on modified media were found to be higher compared to standard media.

Morphological and rheological properties of modified bacterial cellulose were investigated to find out possible differences to the standard cultivation technique.

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GENOMIC AND PHENOTYPIC ANALYSIS OF *RHODOSPIRILLUM RUBRUM* – WILD TYPE AND MUTANT STRAIN

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Rhodospirillum rubrum, a Gram-negative bacterium, is one of the most significant producers of polyhydroxyalkanoates (PHA), which are biodegradable and biocompatible polymers naturally produced by various microorganisms as a way to store carbon and energy. However, genome-wide regulation and transcription in *R. rubrum* are not well described. Therefore, the genomic and phenotypic analysis of the wild type (WT) and the mutant strain (MS), constructed by disrupting two genes coding PHA polymerase, was performed.

Firstly, the culture growth of WT and MS on SYN medium with acetate and then with fructose was measured. From defined time points, the samples were taken, and the RNA-Seq was performed to enable transcriptome comparison. For this purpose, Illumina NextSeq500 was used, and as a result, 75 bp long single-end reads were obtained. Samples obtained under the mentioned culture conditions, each in at least three replicates, were sequenced. The differential expression analysis using DESeq2 was used to identify regulated genes, and moreover, the expression of selected genes was shown using heatmaps.

Secondly, the variant calling of the MS was conducted to identify the causes of phenotypic changes. For this purpose, the mutant strain was sequenced using Illumina MiSeq producing 250 bp long paired-end reads. The reads were trimmed using Trimmomatic and mapped by BWA to the last available assembly of the *R. rubrum* genome (GCA_019134555.1). After reads filtering and deduplication by Picard Tools, the variants in the mutant strain were called with GATK. False positive calls and variants that were underrepresented in the population or had low coverage were filtered out. The remaining variants were further analysed to determine whether they occur in coding regions and, if so, how they affect the phenotype.

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CHITIN-DEGRADING ISOLATES POTENTIALLY USABLE AS THE BASIS OF A BIOPREPARATION

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The development and application of biopreparations are currently key environmentally focused projects to minimize the negative impact of human activity on the environment. The registered preparate must not be phytotoxic, must effectively protect the plant from phytopathogens and/or promote its growth. In other words, it must have biopesticide and/or biostimulant effects. The active ingredient may be prokaryotic (e.g., genera *Pseudomonas*, *Bacillus…*), eukaryotic microorganism (e.g., genera *Trichoderma*, *Pythium…*) and/or their biologically active metabolites.

In this study, a mixed culture of bacterial isolates was isolated from compost. The following work was focused on the basic testing of their potential to be an active ingredient of the biopreparation. The isolation process was carried out as an enrichment culture in the presence of shrimp exoskeletons as inexpensive, chitin-containing waste material served as additional carbon, energy, and nitrogen source. Isolates were further tested for their growth on three carbon and energy sources. All isolates must not be phytotoxic, and therefore this property was also tested using lettuce seeds sensitive to toxic substances. The production of hydrolytic enzymes was studied using diagnostic media and stripes API ZYM® together with fluorometric and spectrophotometric methods. The research was mainly focused on production of chitinases including their kinetics.

Eight individual procaryotic isolates were obtained, namely: *Pseudomonas brenneri* (2x), *Pseudomonas gessardii* (3x), *Arthrobacter stackebrandtii*, *Glutamicibacter uratoxydans* and *Stenotrophomonas maltophilia*. All isolates were non-phytopathogenic and glucose was the most suitable source of carbon and energy. The enzyme profile of *A. stackebrandtii* with the highest biomass growth was the most diverse and rich in proteases, esterases and other hydrolases. Although the highest chitinase activity was fluorometrically determined in the case of one strain *P. gessardii*. The resulted data will help with the selection of isolates for their potential to be a suitable base for a biopreparation with biopesticide and/or biostimulant properties.

ISOLATION AND STRUCTURAL ANALYSIS OF POLYSACCHARIDES FROM CELL WALLS OF GREEN MICROALGAE

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Polysaccharides found in the cell walls of green microalgae have attracted attention for their potential use in the food industry and other fields. We obtained polysaccharide fractions from the cell walls of heterotrophic mutant microalgae *Chlorella vulgaris* H14 and *Parachlorella kessleri* HY1 by successive extractions with hot water and alkaline solution. The extracts were purified using pepsin and hydrogen peroxide to remove proteins and dyes. Polysaccharide fractions were analyzed using elemental analysis, spectroscopic (FT-IR and NMR), and chromatographic (GC-FID) methods. The monosaccharide composition of the polysaccharides varied depending on the type of microalgae and the extraction method used. Hot water extracts contained branched α-L-rhamnan, but galactose was present in different cyclic forms: galactopyranose in the case of *C. vulgaris* H14 and galactofuranose in the case of *P. kessleri* HY1. The spectroscopic analysis confirmed that (1→4)-β-D-glucuronan was the main polysaccharide component of the alkaline extract from the cell walls of *C. vulgaris* H14. Differences in the composition and structure of the cell walls of green microalgae suggest phylogenetic features unique to the Chlorellacea genera, highlighting the potential of these microalgae as a source of specific polysaccharides.

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IN SITU STUDY OF PIGMENTS IN METABOLICALLY VERSATILE BACTERIUM *RHODOSPIRILLUM RUBRUM*

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The presence of pigments such as carotenoids accompanying chlorophyll is very common in most organisms, especially plants and microorganisms (cyanobacteria, purple non-sulphur bacteria etc.) with the ability to photosynthesis. To understand metabolic processes, the connection with production of pigments and qualification of them in cells is very important. The pigments play important role in the defence of the microorganisms to excessive irradiation and increase light absorption simultaneously. Moreover, pigments strongly interact with reactive oxygen species and serve as radical quencher and antioxidant. Therefore, the sudden changes of content or structure of pigments may mean the damage of the cells.

In our study, we focus on *in situ* characterization of specific pigments which are synthetized by bacterial strain *Rhodospirillum rubrum.* However, the pigments are not separated from each other, but they form complexes and interact to each other and with other substances in cells. Accordingly, to our purpose, firstly we quantified the content of pigments in cell. Then we analysed and compared extracted pigments and non-disrupted cells by various spectroscopic techniques such as UV-Vis spectrophotometry measured in regular transmission measurement mode and also in a spatially integrating mode. To evaluate the best combination of methods for monitoring changes and content of each pigment, we also include to our used methods fluorescence spectroscopy to achieve 3D spectra (excitation versus emission spectra). This combination of techniques showed high potential to be exploited in characterization of pigments *in situ.*

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DISTINCT PATHWAYS OF GUAIACOL OXIDATION – THEORETICAL STUDY

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Guaiacol (2-methoxyphenol) can be considered one of the simplest phenolic compounds. It can be found widely in nature and is a common compound of biomass burning emissions. Its oxidation pathways under pyrolytic conditions, as well as solutions at ambient temperatures, are widely studied to identify intermediates and products of these processes. Some chemical or electrochemical experimental reports suggest that oxidation of guaiacyl moiety leads to the formation of catechol followed by the formation of *ortho*-quinone. In literature, there can be found various suggested pathways of guaiacol oxidation involving dissociation of methoxy OCH_3 and hydroxy OH groups. Therefore, we decided to perform theoretical study of thermochemistry of various radical processes leading to *ortho*-quinone or 1,3-benzodioxole formation in gas phase, benzene, and water.
Theoretical calculations of total enthalpies were performed using Gaussian 16 program package. From obtained total enthalpies we calculated individual reaction enthalpies of four relevant mechanisms of guaiacol oxidation. Found results confirm that O–C bond of methoxy group is significantly weaker and more prone to dissociation than phenolic O–H bond in all studied environments. In aqueous solution, weakly acidic OH group can be deprotonated. In phenoxide anion of guaiacol, we observed the lowest enthalpy of $O–CH_3$ group dissociation. These results may lead to a better understanding of the role of the methoxy groups present in naturally occurring compounds, especially in primary naturally occurring antioxidants.

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THE ROLE OF *AZOTOBACTER VINELANDII* AS A BIOINOCULANT AND ITS CAPABILITY OF BIOPOLYMER PRODUCTION AND BIOLOGICAL ACTIVITIES

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Azotobacter vinelandii is a plant growth-promoting bacterium (PGPR), capable of synthesizing two completely different biopolymers with great application potential. Polyhydroxyalkanoates (PHAs) are produced and stored in the form of intracellular granules, while alginate is produced extracellularly and used for bacterial protection. Besides the biopolymers' production, *A. vinelandii* shows biological activities for the stimulation of plant growth, thus it can be used as a bioinoculant.

Bioinoculants enrich the soil in nitrogen and phosphorus levels, decrease pathogens, produce phytohormones, help with phytoremediation by chelating heavy metals from the soil, retain moisture *etc*. These bioinoculant properties lead to a better quality of soil, and the improvement of crop growth and yield. Furthermore, bioinoculants can be used as a biological alternative to chemical fertilizers.

In this work, we screened various effects of plant growth stimulations by the bacterium *A*. *vinelandii*. The tests for the production of phytohormone auxin (indole acetic acid), iron-chelating siderophores and phosphate solubilization showed positive results, resulting in a new generation of bacterial inoculants encapsulated in hydrogel-based carriers.

POTENCIAL OF ENHANCED MICROBIAL METHANOGENESIS IN THE CZECH REPUBLIC

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Coal seams contain large amounts of gas which remains trapped inside until it is released during coal mining or vented to the surface by drilling. Coalbed methane (CBM) represents a significant portion of the world's natural gas reserves, and it has been suggested that up to 20% of the world's natural gas, including CBM, is microbial in origin. Active and abandoned mines are a significant source of coalbed gas, comprising between 30% and 70% of methane. One of the sub-objectives of the project TK01030054 supported by the TA CR was to characterise the key parameters for CBM production in the selected coal mines of the Czech Republic. The gas samples were analysed for chemical composition by gas chromatography (GC-TCD-FID) and for carbon isotopic composition of methane or higher gaseous hydrocarbons by IRMS. Microbial diversity in mine water and coal (brown and hard coal) samples was assessed by molecular genetic methods (q-PCR, DGGE, NGS). Data from detailed analyses of chemical composition and gas and carbon isotope composition, as well as the results of genetic analyses, have provided a number of new insights into the nature and genesis of methane in mine gases. Based on the data obtained, a model was proposed that is able to predict whether microbial methanogenesis occurs under given site conditions (physical, chemical, biological).

POLYNOMIAL FEEDING STRATEGY DURING AN AEROBIC HIGH CELL DENSITY FED-BATCH CULTIVATION AS A TOOL TO INCREASE QUALITY OF THE DRY ACTIVE WINE YEAST

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Fed-batch cultivation is one of the widely used approaches in obtaining yeast biomass. For maximum yield, it is important to choose the optimal growth medium and the feeding rate of glucose and other nutrients during the fed-batch process. Concentration of glucose as low as 0,5 - 1 g/l in the medium lead to repression of respiratory enzymes (the so-called Crabtree effect), i.e. fermentation under aerobic conditions, which results in a significant reduction in biomass yield. During the optimization of fed-batch cultivation of wine yeast, a polynomial feeding model was developed. This model respects both the exponential cell division at the beginning of the cultivation as well as the decreasing specific growth rate during the feeding phase of the process due to the accumulation of waste metabolites and increasing cell density. As a result, the yeast cell cycle can be stopped at the end of the cultivation in the G_0 phase. This ensures a low percentage of budding cells, which positively affects the viability of the yeast after drying and its shelf life in both dry and wet biomass. Furthermore, the model can be easily adapted to a specific wine strain without knowing the exact growth characteristics, simply from the determination of the optical density of cells in the inoculum used to inoculate the bioreactor. This model was tested on 30 wine yeast strains, with an average of concentration 40 g/l dry biomass at the end of the cultivations. The average yield coefficient was 0,46 and the number of budding cells was 7 %, which was also reflected in a longer shelf life and a higher content of the storage carbohydrate trehalose.

THE EFFECT OF ADDED GREEN SOLVENT ON TYROSOL β-D-GALACTOSIDE SYNTHESIS BY FUNGAL β-GALACTOSIDASE

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Tyrosol is a naturally occurring biophenol found in olives, olive oil, and wine with many health benefits. Tyrosol β-D-galacoside provides better bioavailability than pure tyrosol and has the potential to be used as a drug precursor. Enzymatic glycosylation catalyzed by β-galactosidase is the preferred preparation method, as it has full control of the anomeric carbon configuration, takes place under mild conditions, and is low in energy demand. The transfer of galactosyl from lactose to tyrosol is carried out by the transglycosylation mechanism, where the enzyme simultaneously acts as both a transferase and a hydrolase. The result is a kinetically controlled synthesis of a product that is simultaneously hydrolyzed. The product yield strongly depends on the source of the enzyme and the reaction conditions. The reaction conditions can be modified by adding a suitable solvent. Recently, the emphasis has been on reducing the environmental impact of chemical production, therefore this work focuses on the effect of green non-toxic deep eutectic solvents (DES) on the formation of tyrosol β-D-galactoside. First, the effect of DES addition on the initial rates of transglycosylation and hydrolysis was studied. DES composed of betaine and urea proved to be the most effective in reducing the hydrolytic activity of the enzyme, while the transglycosylation activity remained unaffected. The influence of DES was then investigated during the six-hour course of the synthesis. Although the addition of the investigated DES did not bring the expected increase in yield, the study of the initial reaction rates provided valuable information on the preference of the enzyme toward individual acceptors of the galactosyl moiety.

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SKLÍZENÍ JEDNOBUNĚČNÝCH ŘAS POMOCÍ OLEJOVÉ FLOTACE A SEDIMENTACE

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Tato práce se zabývá sklizní zelené jednobuněčné řasy *Chlorella vulgaris* pomocí nového flokulačního činidla připraveného z roztoku hexadecyltrimethylamonium bromidu (CTAB) o počáteční koncentraci 1 g/l a emulze řepkového oleje ve vodě. Molekuly CTAB se vážou na povrch kapiček oleje a vytvářejí kladný náboj částic emulze. Takto stabilizované kapičky emulze za vhodných podmínek (pH, dávka flokulačního činidla) velmi dobře interagují se záporně nabitými buňkami řas, což způsobuje tvorbu vloček a sedimentaci nebo flotaci.

V experimentech byla testována suspenze řas v čerstvém minerálním médiu při různých hodnotách pH a dávkách flokulačního činidla. Z výsledků bylo zjištěno, že pH a množství flokulačního činidla mají významný vliv na účinnost procesu separace řasové biomasy, která při pH 10 a 12 dosahovala vysokých hodnot nad 95 %, a to již při dávce 1,75 ml flokulačního činidla. Získaná biomasa měla navíc v případě účinného procesu relativně nízkou koncentraci CTAB, což by nebránilo jejímu následnému potravinářskému využití. Po prvních pokusech byl obsah CTAB v činidle snížen a pro posouzení vlivu samotného minerálního média byly pokusy opakovány v modelovém médiu NaCl o stejné iontové síle. Pro simulaci reálných podmínek byl použit bovinní sérový albumin a organická řasová hmota. Přídavkem těchto sloučenin došlo k nárůstu dávky emulze potřebné k dosažení účinnosti nad 95 %. Kromě řepkového oleje byly testovány také slunečnicový, olivový a arašídový olej.

ADHESION OF *PYTHIUM OLIGANDRUM* TO MODEL SURFACES

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Pythium oligandrum (PO) is a filamentous oomycete with application as a biocontrol agent, for suppression of plant pathogens in agriculture. During application of commercial product onto plants, one of the important parameters defining the efficacy of its antifungal properties is the adhesion to the plant surface. Attachment to surface can be predicted using thermodynamic approach and DLVO (Derjaguin, Landau, Verwey, Overbeek) theory, and its extended form (XDLVO). In order to make predictions with these models, contact angles and zeta potential of oospores and model surfaces (functionalized magnetic beads) were tested. Thermodynamic model gave basic insight into the predictions of adhesion, while its comparison with DLVO and XDLVO revealed importance of including electrostatic interactions and surface charge in the predictions of adhesion. Additionally, comparison was made between sphere-plate and sphere-sphere models after observation that oospore ornaments were initial contact point of adhesion. Following the predictions, adhesion tests were conducted to study interactions of PO strain CBS109982 oospores, and magnetic beads in pre-defined environments of pH and ionic strength. Predictions between the models varied, and adhesion as later seen in tests, was most accurately predicted by sphere-sphere DLVO and XDLVO models, while thermodynamic did not sufficiently describe adhesion.

REDIRECTION OF METABOLIC FLUXES IN *CLOSTRIDIUM BEIJERINCKII* AS A RESPONSE TO LIGNOCELLULOSE INHIBITORS

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Lignocellulose biomass represents a promising renewable source of utilizable saccharides for biotechnologies upon hydrolysis. Any efficient treatment of this recalcitrant material leads inevitably to the production of chemicals that hinder cell growth or production. Solventogenic clostridia such as e.g. *Clostridium beijerinckii* are able to transform a range of inhibitors and growth in their presence, nevertheless, changes in product ratio to the disadvantage of solvents are a frequent undesirable phenomenon. Seven common inhibitors (vanillic acid, 4-hydroxy-benzoic acid, syringaldehyde, coumaric acid, ferulic acid, furfural and hydroxymethyl furfural) were tested and their impact on growth, acids and solvents production were evaluated for *Clostridium beijerinckii* NRRL B-598. At the same time, the ability of the strain to transform the inhibitors was assessed. All inhibitors except hydroxybenzoic acid were degraded or transformed confirming the ability of strain to cope with certain concentrations of inhibitors. A considerable decrease in solvent production under sub-lethal inhibitor concentrations was observed in the presence of syringaldehyde, coumaric acid and ferulic acid, while it was accompanied by a significant increase in butyric acid formation only in the case of coumaric acid. In the case of ferulic acid and syringaldehyde, rather the ability to fully utilize available glucose was negatively influenced suggesting different mechanisms of impact of inhibitors on fluxes through central metabolism.

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CULTIVATION OF CAROTENOGENIC YEAST ON WASTE POULTRY FAT WITH ADDITION OF COBALT AS A STRESS FACTOR

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Carotenogenic yeast are group of yeast known for production of yellow-red pigments called carotenoids. Red-pigmented yeast are also known for production of immuno-active beta-glucans within their cell walls. Industrially interesting is also their ability of accumulation of high amount of lipids as well as of production of many lipid-soluble compounds such as provitamin D (ergosterol) and coenzyme Q (ubiquinone). Thus, carotenogenic yeast strains are very promising for pharmaceutical or food industry. Due to their high adaptability they can grow within harsher conditions of artificial media with waste substrates. This research is aiming for usage of combination of waste poultry fat and purified glycerol as carbon sources in media and cobalt in the form of Co^{2+} as terminal stressor added in exponential phase of growth to achieve substantial biomass growth and metabolite production. This method of cultivation was tested on genus *Sporidiobolus pararoseus* which achieved higher biomass growth on media with waste poultry fat (22,4 g/l) than on control with glycerol as carbon source. The best growth of biomass was recorded in media with poultry waste fat with addition of cobalt in exponential phase (25,4 g/l). The main goal is the completion of screening phase of experiments where more of genera, such as *Rhodosporidium*, *Rhodotorula* or *Cystofilobasidium,* will be tested and the best cultivation conditions will be subjected to scale-up process into laboratory bioreactor.

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THE EFFECT OF DIFFERENT PLUM VARIETIES ON THE COMPOSITION AND ORGANOLEPTIC PROPERTIES OF SPIRITS

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Fruit spirits are globally popular alcoholic beverages and are usually made from fruits, that are abundant in a given region of the world. The composition of the different species and varieties of fruit grown in different regions varies more or less due to different agrotechnical conditions and differences in genomes and the composition of the fruit is one of the main factors influencing the final composition of the spirits. This study compares the analytical profiles of plum distillates produced from four different plum varieties: Presenta, Valjevka, Čačanská lepotica and Čačanská rodná. The chemical analysis, which was carried out by GC-FID, was supplemented by sensory evaluation and the relationships between production technology, composition and organoleptic properties of the plum distillates were discussed. A correlation between the relatively high content of some substances, such as geraniol, and a positive rating for organoleptic properties and, conversely, a correlation between the relatively high content of some substances, such as 1-propanol, and a worse sensory assesment results were observed. Geraniol and other compounds with pleasant aroma and low perception threshold concentrations could serve as markers of the suitability of a given raw material for production of high quality spirits.

BIOTECHNOLOGICAL CONVERSION OF WASTE FOOD SUBSTRATES BY SELECTED CAROTENOGENIC YEASTS

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The high increase in the human population is associated with a proportionally increasing amount of food waste and raw materials that mankind produces. These wastes still have potential that can be used for biotechnological valorisation. This work focuses on the biotechnological processing of waste oils/fats and waste glycerol by carotenogenic yeasts, which are excellent producer of carotenoids, ergosterol, beta-glucans and other valuable compounds. Results show, that selected yeast strains were able to process waste glycerol as well as some oils and fats in a circular economy model and, moreover, are resistant to potential antimicrobial compounds present in the medium. The best-growing strains *Rhodotorula toruloid*es CCY 062-002-004 and *Rhodotorula kratochvilovae* CCY 020-002-026, were selected for fed-batch cultivation in laboratory bioreactor in a medium containing a mixture of coffee oil and waste glycerol. The results show that both strains were able to produce more than 18 g of biomass per litre of media with high content of carotenoids (10.757±1.007 mg/g of CDW in *R. kratochvilov*ae and 10.514±1.520 mg/g of CDW in *R. toruloides*, respectively). The overall results prove that combining different waste substrates is a very promising option for food wastes valorization and production of enriched yeast biomass.

COMPARATIVE GENOMIC ANALYSIS OF TWO *SCHLEGELELLA* SPECIES BRINGS NOVEL INSIGHTS INTO POLYHYDROXYALKANOATES PRODUCTION

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Polyhydroxyalkanoates (PHAs) are biodegradable and renewable polymers synthesized by many bacteria under nutrient-limited conditions. *Schlegelella thermodepolymerans* and *Schlegelella aquatica* are capable producers of PHAs with promising characteristics for industrial applications. Genus *Schlegelella* covers several species and has so far two synonyms, *Caldimonas* and *Caenibacterium*, providing new opportunities for the exploration of genomic features using additional species currently classified outside the genus under study. Understanding the regulation of PHA production in these bacteria is crucial for improving PHA yield. However, the regulatory mechanisms are still poorly understood.

Here, we report the identified key elements involved in PHA biosynthesis and the comparison between strains *Schlegelella thermodepolymerans* DSM 15344^T, DSM 15264, LMG 21645, and *Schlegelella aquatica* LMG 23380^T. Through genome sequencing and analysis, we found that the PHA biosynthetic pathway in these bacteria is regulated by a complex network of genes, including *phaC*, *phaA*, *phaB*, *phaR*, *phaP*, and *phaZ*. In addition, our attention was directed towards the control of sugar metabolism, and we discovered a unique regulatory mechanism responsible for the utilization of xylose among the bacteria examined.

Our findings provide insights into the genetic basis of PHA biosynthesis in these bacteria and lay the foundation for further genetic engineering to improve PHA production in the genus *Schlegelella/Caldimonas*. These results have important implications for the development of sustainable bioplastics and the mitigation of plastic pollution.

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DECARBONISATION AND THE ECONOMICAL ASPECTS OF THE CHEMICAL INDUSTRY TRANSFORMATION

IS GREEN HYDROGEN COMPETITIVE?

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Hydrogen production is on a rise every year, but the main issue with this is that it is produced majorly via steam methane reforming method (around 96% of the total hydrogen production). This methodology utilises natural gas a feedstock for the production of hydrogen which is still environmentally detrimental given it produces on an average around 7 kg of carbon dioxide per kilogram of hydrogen produced. The most environmentally friendly and sustainable form of hydrogen is green hydrogen, which is produced via electrolysis of water, and using renewable energy sources as feedstock for electricity requirement like solar energy and wind energy. The issue with green hydrogen is the economic viability and commercialisation of the production equipment like electrolysers. Review of the economic viability of the green hydrogen by using financial tools contributes to the right investment decisions. Sensitivity analysis is to changed input variables like electricity prices, selling price of green hydrogen and CAPEX investment provides a better picture of the entire investment process. A comparison with steam methane reforming is performed to come forward with a result which can present the economics behind the green hydrogen production price. The price at current production cost level at 5,5 EUR/kg can be competitive to the price of hydrogen produced via steam methane reforming hen proce of natural gas (methane) is higher than 100 EUR/MWh (see Figure 1).

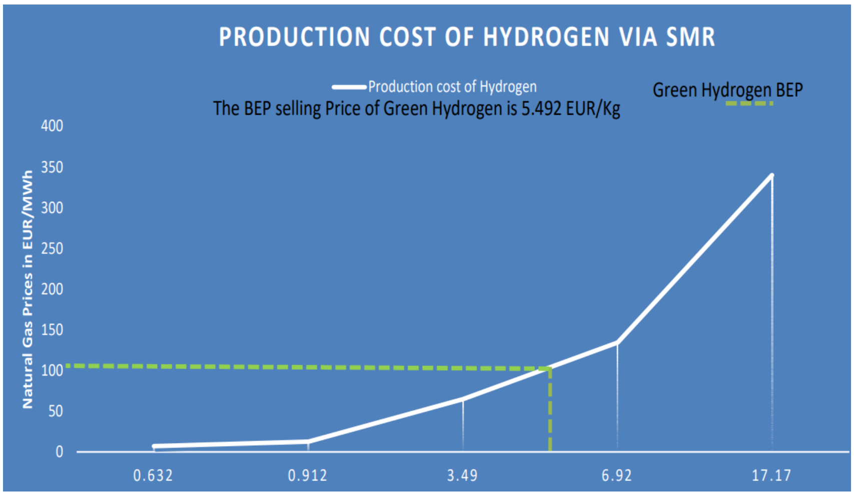

Figure 1: Production cost of hydrogen via SMR with marking of selling price (BEP) of green hydrogen

CCU SOLUTIONS VS. ADDITIONAL ENERGY REQUIREMENTS

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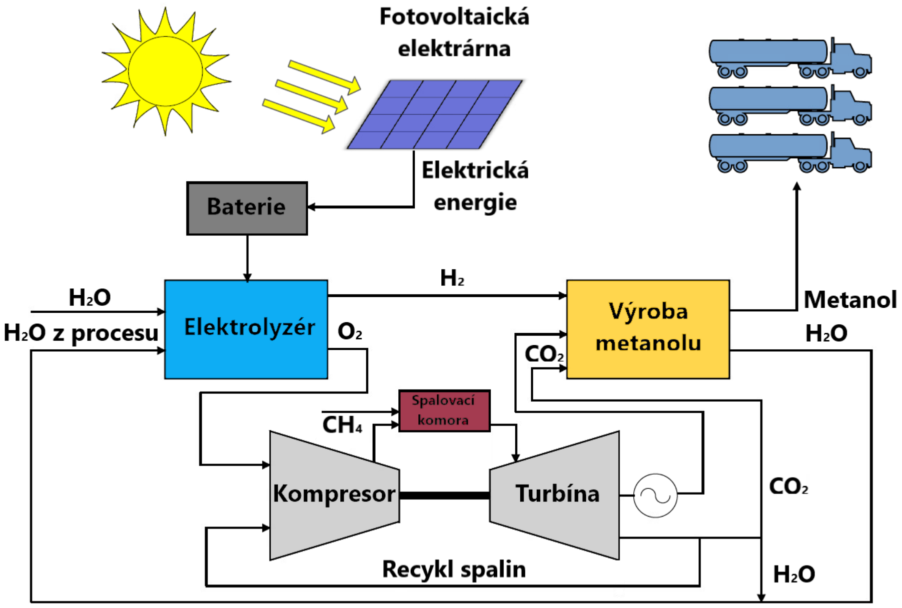
The issue of global warming and the role that fossil fuel emissions are playing is subject of political and technical disputes. This work is demonstrating the concept of elimination of CO2 emissions from small gas turbine with capacity of 0,3 MW consuming 3,5 kt of natural gas per year and emitting 9,5 kt of CO_2 per year. This amount of CO2 could be converted to 6,9 kt methanol per year.

In order to convert CO2 to methanol, the green hydrogen production should be established. The amount of green hydrogen needed for defined quantity of methanol is about 1,3 kt/y. This amount of hydrogen could be produced by electrolyser with installed capacity 10 MW!

The interdependence of balance of production streams (water, hydrogen, CO_2, oxygen for gas turbine operation and methanol) was analysed and balance model has been developed.

This work identifies that green solution are significantly dependent on large amount of green electricity. Nevertheless, this concept could be used in situations of large access of the electricity from renewable sources converting CO2 it into products for final use or accumulating energy into products which are easy to store.



OPTIMIZING STEAM POWER IN INDUSTRY– DECARBONIZATION OPPORTUNITY

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Mechanical energy in refineries and in heavy industry generally, can be provided either by electromotors or by steam drives, the latter serving for decades as favorable solution wherever cheap steam was available. With rising fuel prices, tightening emission limits, rising carbon tax and recent trends of electrifying industry, the economics of steam drives operation is considered questionable. Its reevaluation should be performed in the wider balance frame of the whole industrial enterprise or industrial cluster. Steam production facilities as well as steam pipelines operation are both affected by potential switch from steam power to electropower. If less than required attention is paid to these aspects, electrification projects may face delays and be burdened by extra costs related to tight spots occurrence in steam systems. Whether be it undersized of oversized steam pipelines resulting from steam mass balance change followed by worsened delivered steam quality, or unfavorable changes in central steam and power plant operation, all that may lead to a reduction in the achieved electrification benefit. A deeper insight in steam pipelines operation and heat and power production in industry is desirable, to address the potential issues resulting from switching to electropower. This contribution presents the adopted approach and the main results of modeling the steam pipeline network in a refinery in multiple scenarios considering different variants of condensing steam drives replacement by high-speed electromotors. This work was supported by the Slovak Research and Development Agency, Grant No. APVV-18-0134.

DEKARBONIZAČNÍ PROCESY Z POHLEDU ZÁCHYTU A VYUŽITÍ CO2

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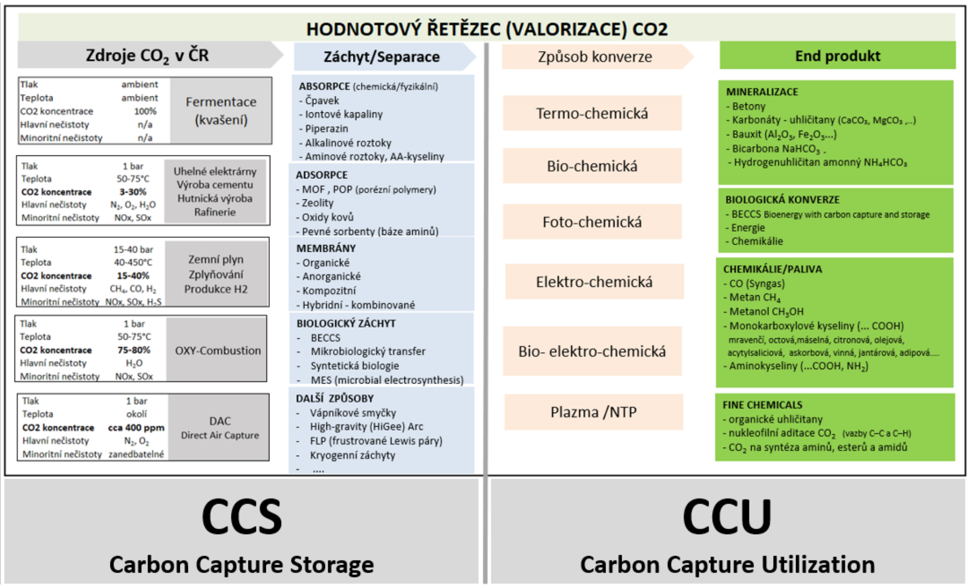
Dnes emise skleníkového plynu CO2 již extrémně zatěžují zavedené výrobní, průmyslové a energetické řetězce, fungující na báze fosilních zdrojů. Ekonomické nástroje EU ETS, Taxonomie, ESG, a směřování evropské a národní legislativy, vytvářejí již v současné době ekonomickou základnu pro dekarbonizaci těchto odvětví, ve smyslu zabránění vypouštění skleníkového plynu CO2 do atmosféry. Navíc, odklonem od využití klasických fosilních zdrojů uhlovodíků (ropa, zemní plyn, uhlí), v blízké budoucnosti, získává tento skleníkový plyn i novou dimenzi zájmu o využití uhlíku z této molekuly. Využití této termodynamicky velmi stabilní molekuly, otevírá celé spektrum nového vědeckého přístupu jak v oblasti záchytu CO2, tak především v oblasti jeho využití jako vstupní suroviny pro výrobu uhlovodíků. Procesy využití CO2 – Carbon Capture Storage & Utilization jsou tak novou výzvou pro výzkum v mnoha vědeckých oblastech – absorpce (chemická a fyzikální), adsorpce, membrány, syntetická biologie, elektro-syntézy, katalytické procesy, plazma,…).



BETTER SAFE THAN SORRY – ARE WE RUSHING HYDROGEN?

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Hydrogen is considered both an energy vector and an energy store for the near future. Its conventional production by steam reforming is burdened with severe environmental impact. On the other hand, low-carbon alternatives of hydrogen production have either high energy intensity or low technology readiness level associated with higher risk. The situation is even worse when considering source of the energy required for "green" hydrogen production pathways.

In this work, different hydrogen production routes based on well-established steam reforming and modern electrolysis are investigated. To assess overall environmental impact, analysis of emissions from different energy sources is conducted as well. For electricity, current and future grid mixes are examined as well as in-house electricity production from renewables. Similarly for heat source, conventional and low-carbon alternatives are analyzed.

The results suggest necessity of blue hydrogen production as an intermediate step in transition towards green hydrogen generation via electrolysis. Estimates of costs and carbon footprint of each analyzed production route will be presented too. Suggestions for sustainable hydrogen production in conditions of Slovak Republic are formulated as a part of the contribution.

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LOGISTIKA V CHEMICKÉM PRŮMYSLU

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Logistiku lze chápat jako podpůrnou disciplínu, která se přímo nepodílí na hlavní výrobě, ale zásadním způsobem jí ovlivňuje. Pro správně fungující produkční systém jakéhokoliv typu je správně fungující logistika klíčová (ovlivňuje zejména množství prostojů, rychlost výroby, kvalitu výroby a velkou měrou i nákladovost výroby a nároky na množství kapitálu vázaného v zásobách). Další důležitou úlohou logistiky je transformace rozdílů mezi produkcí výrobce a spotřebou zákazníka v místě, čase a množství. Logistika v chemickém průmyslu je navíc spojená s řadou specifik jako např. přeprava a skladování hořlavých a nebezpečných látek, které si vyžaduje zvláštní režim a bezpečnostní opatření. Nebo fakt, že těžký chemický průmysl vyrábí vstupní materiály pro jiné výrobce a tudíž jde o obchodní a marketingový koncept B to B (B2B). Pravděpodobně nejdůležitější vstupní surovinou pro chemický průmysl je ropa. Je to klíčová surovina, pro fungování jakéhokoliv národního hospodářství průmyslově rozvinutého státu. Problém je, že její naleziště na světě jsou situována velmi nerovnoměrně, z čehož plyne nutnost jejího transportu v obrovských objemech na velmi dlouhé vzdálenosti. Zajímavostí je, že v řešení tohoto problému v celosvětovém měřítku nedominují ropovody, ale tankery. V r. 2000, dávno před vypuknutím konfliktu na Ukrajině, kdy se do Evropy dováželo velké množství surovin z Ruska byl ropovod Družba transportující ropu ropovod s největší kapacitou na světě, která činila 1,4 milionů barelů denně. Což je zlomek oproti číslu 17 milionů barelů denně, což je množství ropy, které bylo ve stejném roce transportováno pomocí námořních tankerů z oblasti Perského zálivu do Asie a USA.

V našem článku chceme analyzovat některé nové vývojové trendy v logistice se zřetelem na logistiku spojenou s chemickým průmyslem včetně poukázání na význam námořní přepravy v mezinárodní logistice a celosvětovém obchodu.

MOŽNOSTI IMPLEMENTACE PRINCIPŮ CIRKULÁRNÍ EKONOMIKY V MALÝCH A STŘEDNÍCH PODNICÍCH CHEMICKÉHO ODVĚTVÍ V ČR

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Úvod

V souvislosti se zaváděním udržitelných postupů a řešení do podnikové praxe se do popředí zájmu dostávají nová témata, mezi která patří i cirkulární ekonomika. Jejím cílem je snížení spotřeby přírodních zdrojů v ekonomice, založena je na principu uzavírání či cirkulaci toků uvnitř výrobkových a materiálových systémů, a to i se zohledněním ostatních aspektů udržitelného rozvoje. K dosahování cílů cirkulární ekonomiky byly vyvinuty tzv. R-strategie, či „rámce R“. Mezi nejběžnější patří 3R: Reduce, Re-use, Recycle, tyto byly postupně doplňovány strategiemi, jako je Refuse, Rethink, Repair, Refurbish, Remanufacture, Repurpose, či Recover. Přechod na cirkulární ekonomiku tak vyžaduje inovace, nové obchodní modely či sociálně-institucionální změny, zaměření se již na fázi návrhu výrobku a hodnocení všech fází životního cyklu produktu. Tento příspěvek shrnuje výsledky výzkumu, jehož hlavním cílem bylo zjistit, jak jsou tímto novým směrem ovlivněny malé či středně velké podniky, jaké aktivity v této oblasti implementují, jaké jsou důvody zavádění principů cirkulární ekonomiky do jejich činnosti, jakým čelí překážkám, či jaká vnímají ohrožení, ale i příležitosti. Konkrétně byly vybrány podniky odvětví chemického průmyslu. Výzkum byl zpracován pomocí metod kvalitativního výzkumu zahrnující osobní dotazování a diskuse se zástupci vybraných firem.

INITIAL ANALYSIS OF INTEGRATION OF HEAVY RESIDUES GASIFICATION PLANT INTO OIL REFINERY AS A POSSIBLE WAY OF INDUSTRY DECARBONISATION

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An integrated gasification plant fulfils partly the role of industrial steam and hydrogen plants by polygenerating valuable products (hydrogen, power, steam) from low-value products. Carbon-energy-economy analysis (or CEE analysis) is a possible means of conceptual techno-economy evaluation of such processes. Integration of heavy residues gasification plant into medium size oil refinery is modelled in this study. It is expected to lead to reduced consumption of natural gas in the refinery and to lower overall carbon dioxide emissions. Case studies with different summer and winter mode of operation, before and after integration, are assessed and compared by consumption of electricity, natural gas and heavy residues, as well as by CO_2 emissions, by capital- and operational expenses and by the estimated payback period. Integration of gasification plants within industrial enterprises and clusters and their optimisation shows more promising than constructing standalone plants and might have a positive environmental, energy and economy impact. This conceptual analysis is a good starting point to deeper techno-economy analysis and multi-level optimization with respect to minimization of integrated plant´s payback period, construction costs, and energies consumption and losses as well.

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EFFECTS OF ELECTRICITY GRID MIX ON CARBON FOOTPRINT OF CARBON CAPTURE AND STORAGE IN HYDROGEN PRODUCTION

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Hydrogen is becoming one of the most valuable substances in the world. During his production by steam methane reforming, significant amount of carbon dioxide is emitted. In the fight against climate changes, we are investigating how to decrease its emissions. We were focused on post-combustion carbon capture as it is the most industrially employed method.

We have designed three units for capturing CO_2 that are based on different separation processes. The first technology based on amine absorption (AA) where we capture 90 % CO_2 with 98 % purity. The second, membrane separation (MS) where we capture 80 % CO_2 with 95 % purity. As the third option, we have added oxy-fuel combustion (OFC). From the capture perspective, we can separate practically whole CO_2 content from the flue gas and generate CO_2 stream of 99 % purity.

However, to calculate carbon footprint of our process, we cannot neglect additional amount of CO_2 emitted from energy consumption. In our processes, electricity is used for compression and pumping while in case of absorption, heat for reboiler is needed as well. The additional amount of CO_2 that is emitted during the generation of these energy stocks is highly dependent on the source which it is produced from. From fossil fuel power plants without carbon capture (CCS) the CO_2 emissions are the highest. For example, from pulverized coal power plant (PC) without CCS it is 0.973 kg CO_2/kWh electric energy, from natural gas power plant 0.44 kg CO_2/kWh e.e. and from nuclear power plant only 0.005 kg CO_2/kWh e.e. The power plants that use renewable resources like solar, hydro or wind energy, play a significant role as well.

In some instances, we are able to produce our own electricity from one source, but generally this is not an option (specifically for higher energy demands). In that case we have to take it from the grid where is the electricity mix from different sources. We have found out that taking into account CO_2 emitted for energy production, overall efficiency of carbon capture is lower by 18 % in absorption, 5 % in membrane separation and 4 % in oxy-fuel combustion. PC without CCS provides the worst option as 19 % in AA, 42 % in MS, and 25 % in OFC of captured CO_2 is emitted by electricity generation. On the other hand, the most promising solutions are renewable resources or nuclear energy where the percentual degree in efficiency is the lowest.

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COMPARING ACTUAL SIMULATION DATA WITH LITERATURE ASSUMPTIONS – CASE STUDY OF OXYGEN PRODUCTION FOR OXY-FUEL COMBUSTION

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With increasing socio-environmental demands on industry, the costs associated with emissions are rising, so there is a need to look for options to reduce them effectively. The main component of emissions is carbon dioxide, the production of which is associated with most chemical processes involving carbon. Industrial companies are encouraged to solve this problem, while the current trend is to capture it. Carbon dioxide can be used to produce chemicals, such as methanol or synthetic natural gas, thus using the energy potential of this originally waste stream. In this work, carbon dioxide was captured from hydrogen production by steam methane reforming, where it is produced as a by-product in significant quantity. There are several ways to capture carbon dioxide and potential one of them, oxy-fuel combustion, was examined. In this process, nitrogen is not introduced in the combustion and carbon capture which makes the capturing process technologically easier. However, an important raw material for this process is high-purity oxygen. In practice, cryogenic air separation unit (ASU) is commonly used for oxygen production, which is an energy-intensive process. For this reason, an ASU was added to the simulation to be able to evaluate the economic as well as the energy intensity of the whole process. The data obtained from the developed model were compared with literature assumptions characterizing the ASU, mainly the specific electricity consumption for the oxygen production. When comparing the unit price of hydrogen produced for our system with the literature, the impacts of the unit lifetime and the sale of ASU by-products were identified as crucial. Besides economic analysis of both hydrogen production and carbon dioxide capture costs, emissions directly and indirectly associated with production were quantified. The carbon capture process and the operation of the ASU is energy intensive; comparison of two possible alternatives were made. The use of grid and emission-free green electricity were compared through economic and environmental point of view.

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OPERANDO DRIFTS SETUP FOR THE COMPLEX STUDY OF CO_2 HYDROGENATION OVER MXENES

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Nowadays, one of the biggest global environmental issues is CO_2 valorization, which is rather demanding due to the high thermodynamic stability of CO_2 molecules. The valorization is crucial not only for the efficient reduction of CO2 emissions but the CO2 conversion can also provide important market products like synthesis gas and methanol in the case of CO2 hydrogenation.

Here, we present an operando DRIFTS setup for the complex characterization of the hydrogenation process. The setup allows the collection of infrared spectra at a wide range of temperatures (from RT to 800 °C) and pressures (up to 10 bars). The gaseous atmosphere around the characterized sample is controlled by a series of mass flow controllers to tune the reaction mixture composition. An inherent part of the DRIFTS setup is sampling of the gaseous reaction mixture in GC/MS instruments.

As a catalyst showcase, we used Niobium MXenes (Nb_2CT_x); a 2D material of the future with predicted high efficiency for CO_2 activation. The attractivity of this new type of material for CO2 hydrogenation stands in reduced utilization of metal(s) and natural high surface area of 2D materials.

This DRIFTS setup provides a complex correlation between the characteristics of the catalyst surface and the amount of produced hydrogenation products at the same time. Furthermore, the setup allows temperature- and time-resolved catalyst characterization.

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ECONOMICS OF THE CHEMICAL INDUSTRY

ZHODNOCENÍ VÝHOD IMPLEMENTACE KONCEPTU CSR V PODNICÍCH

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V důsledku rostoucí globalizace a rostoucího počtu nadnárodních firem, ovlivňujících podnikatelské prostředí, kvalitu života a stav životného prostředí je nutné zajistit, aby firmy dodržovaly základní mezinárodně platné standardy. Navíc roste informovanost a sofistikovanost zákazníků a tím i jejich požadavky na firmy. Také společnost očekává od firem větší transparentnost a informovanost o všem co souvisí s dopadem jejich činností na společnost jako celek. Společensky zodpovědné podnikaní představuje inteligentní vykonávání ekonomické činnosti, jejímž přínosem je zabezpečeni kontinuity firmy z dlouhodobého hlediska. CSR pak představuje široký a globálnější pojem, který může být doplněný o konkrétnější usměrnění v porovnaní s iniciativou Responsible care, agendou REACH anebo normami ISO, které obecně zahrnují soubor definovaných pravidel. Čím víc si firmy uvědomují svoji environmentální a sociální zodpovědnost, tím víc se jejich manažerské postupy vyvíjí směrem k širší implementaci CSR. Manažerské chování a řízení podniku tak respektuje nejen ekonomické a technické zájmy firmy ale i lidská práva, etické chování, zájmy zaměstnanců a ostatních stakeholderů. Do úvahy bere také potřebu péče o životní prostředí, minimalizaci odpadu a podnikovou filantropii. Koncept CSR si za dobu své existence získal skupinu obhájců stejně jako kritiků. Protichůdné názory odborníků se týkají diskuse, zda aktivity CSR opravdu přispívají k trvale udržitelnému rozvoji anebo je to například jen forma reklamy. Někteří odborníci také vnímají udržitelný rozvoj jen jako poloviční řešení na rozsáhlé problémy, kterým nyní společnost a svět čelí. Škody, které byly již způsobeny jsou tak rozsáhlé, že není možné se pouze spokojit s nynější situací a udržovat ji a je nutné přistoupit k regenerativnímu udržitelnému rozvoji. Příspěvek se tak zabývá stále více diskutovanými nejen výhodami ale i nevýhodami CSR a argumenty pro přijetí/nepřijetí společenské zodpovědnosti firem v podnikaní.

WAYS TO IMPROVE THE COLLECTION AND RECYCLING OF SEPARATE WASTE IN THE SELECTED REGION – CASE STUDY

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The global shift towards sustainable behaviour is also affecting waste management practices. Recycling is one way to reduce waste. It allows to apply the principles of circular economy by eliminating the single use of different types of materials. The paper deals with waste collection and recycling in a selected region of the Czech Republic and the possibilities of improving these processes. It presents the results of a primary qualitative research conducted in two phases, first in a company engaged in waste collection and sorting, then in a company implementing the recycling process itself. The research involved the collection of primary information through face-to-face interviews according to an interview scenario, which was complemented by observations. The research was aimed at identifying how to implement both the collecting process (in the first phase of the research) and the recycling process (in the second phase of the research), while identifying tools to improve these processes. The revealed tools can be classified into three basic groups, namely tools for the implementation of technical and technological innovations (concentrated mainly on cost savings), improvement of personnel processes (processes related to recruitment and selection of employees, adaptation processes and processes aimed at increasing work-friendliness) and tools enabling the use of optimization methods and models in the management of in-house processes (including the introduction of appropriate information technologies). The research results and their discussion can contribute to improving collecting and recycling not only in the companies where the primary research was conducted, but also in other companies operating in the Czech Republic. They can also be an inspiration for foreign companies, but only after considering the degree of similarity of the conditions under which companies of this type operate.

INDIKÁTORY UDRŽITELNÉ VÝROBY V CHEMICKÝCH PODNICÍCH

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The growing pressure of the public on the sustainable behavior of companies is causing changes in the product portfolio as well as changes in production processes in all industries. The ongoing digitization of business processes facilitates production, helps monitor production processes and ensures high quality and competitiveness. Chemical production companies are also adapting to the transformation of the industry and, even with regard to the rising prices of resources, they are trying to produce in a sustainable way. The sustainability of production and products needs to be monitored through appropriate indicators. Their use and utilization was mapped by qualitative research in a selected chemical company. The dimensions of sustainability were identified according to the triple-bottom-line concept and the key indicators of production sustainability evaluation were verified in them.

SUSTAINABLE HUMAN RESOURCES MANAGEMENT

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Sustainable development is a concept that has been worked with for many years. However, sustainable human resource management has only appeared in the literature in the last 15 years and in applied form in companies for an even shorter period of time. Due to this, the content of this concept is not yet fully unified. In its broadest sense, it is about managing employees so that the organisation achieves its economic, social, human resources and environmental objectives, both in the short and long term. The narrowest concept is probably allowing employees to undertake volunteer activities of their choice during designated working hours. A slightly different view states that sustainable HRM is about enabling an individual to be employable throughout their working life. Whatever the view, in what is still a very global and highly competitive world, the issue of sustainable human resource management will also have to be faced by chemical companies relatively soon.

This article presents selected Czech results of a major international survey on sustainable development issues. It focuses on comparing the differences found between industrial and service enterprises and suggests basic ways to introduce sustainable human resource management in chemical enterprises. The expected significant difference between industry and services was found to be the offering of telecommuting (p-value = .00035). Surprisingly, on the other hand, industrial enterprises were found to be significantly more likely than services (p-value = .00057) to tie a portion of employee compensation to compliance with CSR objectives.

The research confirmed high employee job satisfaction, but the contingency table tests did not show a relationship between job satisfaction and selected activities that are expected to saturate job satisfaction (e.g., specific programs to facilitate adaptation or corporate training programs).

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ONLINE REPUTATION MANAGEMENT V PODNICÍCH CHEMICKÉHO PRŮMYSLU V ČR

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Příspěvek analyzuje význam a využití vybraných nástrojů online reputation managementu v podnicích chemického průmyslu sdružených ve Svazu chemického průmyslu ČR. Jsou prezentovány výsledky primárního výzkumu mapujícího využití vybraných forem online komunikace podniků se stakeholdery a identifikujícího intenzitu využití různých proaktivních a reaktivních technik řízení reputace sledovaných podniků v online prostředí. Závěrem jsou na základě výzkumu navržena doporučení pro chemické podniky poskytující praktické vodítko, jak aktivně vytvářet a trvale podporovat pozitivní online pověst podniku prostřednictvím placeného a vlastněného obsahu a zároveň monitorovat a reagovat na online získávaný (sdílený) obsah tak, aby byl vyzdvihován žádaný image podniku a zároveň byl minimalizován dopad případné negativní online publicity na reputaci firmy.

CIRCULAR ECONOMY IN ENTERPRISES OF THE CZECH CHEMICAL INDUSTRY
CIRKULÁRNÍ EKONOMIKA V PODNICÍCH ČESKÉHO CHEMICKÉHO PRŮMYSLU

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Abstrakt

Problematika bio-based/cirkulární ekonomiky je v posledních letech zmiňována stále častěji mezi odbornou veřejností i v podnikové praxi. Tato koncepce oprávněně stojí v popředí zájmu právě proto, že představuje jednu z možných cest k dosažení cíle udržitelné budoucnosti. Příspěvek publikuje výsledky kvalitativního výzkumu realizovaného v průběhu roku 2022 ve vybraných podnicích z oblasti chemického průmyslu působících v České republice, shrnuje, jak se tato aktuální problematika promítá do postojů a konkrétních aktivit vztahujících se k BBE/cirkulární ekonomice. Výsledky naznačují, že mezi hlavní oblasti zájmu patří sledování aktuálního vývoje legislativy v ČR a EU, zavádění technologií na snížení energetické náročnosti výrobního procesu a v neposlední řadě respektování požadavků zákazníků v oblasti ISCC.

Abstract

In recent years, topics of the bio-based/circular economy has been mentioned more and more often among the professional public and in business practice. This concept is rightly in the forefront precisely because it represents one of the possible ways to achieve the goal of a sustainable future. The paper publishes the results of qualitative research on the topic of carried out during 2022 in chosen companies from the chemical industry operating in the Czech Republic, summarizes how this current issue is reflected in attitudes and specific activities related to BBE/circular economy. The results suggest that the primary areas of focus are monitoring the current development of legislation in the Czech Republic and the EU, introducing technologies to reduce the energy intensity of the production process and, last but not least, respecting customer requirements in the field of ISCC.

IMPLEMENTATION OF ENERGY SAVING PROJECTS IN CHANGING ENVIRONMENT

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Energy saving efforts lead to increased demand for materials used in projects. Technical solutions require the use of thermal insulations in all sectors of the economy. The demand depends on the decision of the owners about the implementation of the project. The paper compares decision-making based on project evaluation where standard economic criteria are used and on setting goals for energy consumption decreasing during certain time interval. For example, current decision of EC on energy consumption decreasing in existing buildings. These different approaches can substantially change the time dependent curve of projects implementation. The solution, described in the paper, is based on the development of the model describing the dynamic behavior of the system. Exogenous variables are changes of the energy prices and investment costs. Main output parameter is the implementation rate during the observed time interval. The investigated field is the refurbishment of the existing building stock. Another issue connected with this problem is also estimation of needed amount of financial resources.

CURRENT MARKET NEEDS IN CHEMISTRY EDUCATION IN THE FIELD OF BUSINESS AND ECONOMIC INNOVATION

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Current market needs indicate, under the influence of development and the situation in which the company finds itself, the need for reorganization in the field of education at universities. The resulting situation in society and on the labour market creates pressure for the emergence of new competencies for graduates. Therefore, it is necessary for educational institutions to be able to respond in an appropriate way to the needs of the labour market and to adapt the curricula of educational programs to the needs of practice. In the lecture, we will identify a specific market need to expand education in the field of chemistry to a specific field in a state institution, and we will propose a solution in the field of education at the university in the creation of new interdisciplinary study programs.

CHEMICAL PROCESSES AND DEVICES

VELKÁ VÝZKUMNÁ INFRASTRUKTURA ENREGAT...OD ZÁKLADNÍHO PO APLIKOVANÝ VÝZKUM...POKRAČUJE I V LETECH 2023-2026

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Velká výzkumná infrastruktura ENREGAT, představující jedinečnou základnu pro realizaci komplexního výzkumu v oblasti materiálového a energetického využití odpadů pomocí spalovacích, pyrolýzních, anaerobních a katalytických procesů, nabídne díky podpoře ministerstva školství své služby i v následujících čtyřech letech. Nově je od roku 2023 rozšířena nabídka přístrojů a zařízení z ukončených projektů například o skenovací elektronový mikroskop nebo iontový chromatograf s vodivostní detekcí, včetně dalších úprav pro zajištění vysoké znalostní i technologické úrovně poskytovaných služeb.

Velká výzkumná infrastruktura již přispěla ke vzniku 100+ publikací v impaktovaných časopisech. Její využití vedlo ke vzniku pěti patentů a dalších zajímavých aplikovaných výsledků. V rámci otevřeného přístupu bylo schváleno přes 350 žádostí nejen z hostitelské organizace, ale i z českých a zahraničních univerzit napříč kontinenty. Jsme vyhledávanou infrastrukturou také pro pracovníky Akademie věd ČR a SR. Neméně důležitou činností je spolupráce s partnery z aplikační sféry. Realizace na 99 projektech s 54 partnery z aplikačního sektoru přispěla k přeměně výsledků na udržitelná řešení s ekonomickou hodnotou a sociálním přínosem.

„Experimentální výsledky byly získány s využitím velké výzkumné infrastruktury ENREGAT podporované MŠMT, č. projektu LM2023056.“

NOVÉ TECHNOLOGIE V INFRAČERVENÝCH SPEKTROMETRECH DEDIKOVANÝCH PRO MONITOROVÁNÍ PROCESŮ

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Infračervená spektroskopie v blízké (NIR) a střední (MIR, FTIR) infračervené oblasti je široce využívanou technikou nejen v oblasti laboratorních analýz, ale díky přednostem jako je rychlost měření, nedestruktivnost a univerzalita je jednou z nejpoužívanějších technik v oblasti procesního monitoringu – ať už v online, in-line či at-line uspořádání.

V posledních letech byla ve výzkumném centru Bruker Optics vyvinuta celá řada inovativních technologií a tyto technologie byly implementovány do nových procesních spektrometrů. Za zmínku stojí především FT-NIR analyzátor MATRIX-F II s patentovanou konstrukcí vnitřní optiky odolné proti vibracím a mechanickým vlivům, se kterými se optické přístroje v průmyslové výrobě často špatně vypořádávají. Další zajímavou technologií u tohoto přístroje je možnost kombinace většího počtu různě konstruovaných sond na jednom zařízení a to jak, pro pevné látky, tak i kapaliny. Za zmínku stojí především reflexní hlavy pro bezkontaktní měření pevných látek na větší vzdálenost.

Dalšími pokrokovými přístroji jsou dedikované FTIR(MIR) analyzátory plynů, které díky unikátnímu hardwarovému a softwarovému řešení eliminují či potlačují naprostou většinu nedostatků FTIR spektrometrie v této oblasti (nutnost tvorby kalibrací, křížová citlivost, vliv teploty a tlaku). Jde o velmi inovativní zařízení otevírající zcela nové aplikační možnosti všude tam, kde je potřeba rychle a přesně detekovat a kvantifikovat větší množství plynných složek současně.

ZÁŽITKOVÉ VZDĚLÁVÁNÍ V PROCESNÍM INŽENÝRSTVÍ

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Propojení chemického průmyslu s akademickým prostředím v rámci Univerzitního centra VŠCHT – FS ČVUT – ORLEN Unipetrol vytvořilo jedinečnou příležitost k uplatnění zážitkového vzdělávání v rámci výuky chemických a procesních inženýrů. Univerzitní centrum využívá nově vybudované školící středisko v areálu ORLEN Unipetrol, které je vybaveno několika moduly pro školení operátorů, inženýrů a v současné době také studentů. Dále jsou pro výuku využívány laboratorní a poloprovozní aparáty instalované v laboratořích FS ČVUT. Na instalovaných aparátech a technologiích si mohou studenti prakticky vyzkoušet reálné řízení a chování běžně používaných procesů v chemickém či potravinářském průmyslu. V práci jsou prezentovány vzorové příklady zážitkově orientovaných projektů, které se pokouší inspirativně představit potenciál zážitkového vzdělávání v oblasti procesního inženýrství. Vyhodnocením zpětné vazby od studentů bylo prokázáno, že absolvování zážitkových projektů účinně prohlubuje a doplňuje znalosti, dovednosti a zkušenosti studentů. Zážitkové vzdělávání také rozšiřuje motivaci k dalšímu, např. doktorskému studiu.

FLUE GAS CONDESER OF BIOMASS-FIRED HEATING PLANT

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In the Czech Republic, biomass is becoming more and more popular, even in the context of fuel. As part of the fulfillment of European climate plans, the burning of biomass is favored by some programs (green bonuses, guaranteed purchase price) and penalized by others (EU ETS – European Union Emission Trading System). However, biomass in itself is a very comprehensive term and the individual types of biomass differ quite significantly from each other in terms of quality. One of the most discussed types of biomass is wood chips, mainly due to its available quantity.

However, the moisture content of wood chips fluctuates considerably and in some cases reaches a value of up to 50% by weight. The condensation mode of flue gas enables the removal of moisture after the combustion process, while when applying a heat exchanger, the system uses part of the latent heat and generates savings for the company. The contribution deals with the design of condensing technology for the real conditions of boilers burning solid fuels of an industrial partner.

METTLER-TOLEDO SETS UP NEW TECHNOLOGY LEVELS TO CHRYSTALLIZATION STUDIES

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Mettler-Toledo is an instrument supplier with long term experience of in-situ particle characterization and in-situ reaction analysis demands. We know what are the biggest challenges in this fields. We tailor our Process Analytical Technology (PAT) devices towards those challenges to ensure best in class reliability, sensitivity, data evaluations and data platform connectivity.

This presentation will highlight recent developments for the technologies related to crystallization studies. Mettler-Toledo wants to bring best in class instruments available rather than making compromices when trying to connect all instruments to one probe. We understand the challencies of data performance and the fact that data needs to provide highest possible confidence.

The New EasyViewer with New Image2Chords algorithm will justify the demands to characterize partickle size and shape in-situ, i.e. particle size distributions, particle size ranges, mean, median values, e.t.c. over the time. New Easy Viewer system allows user to leave the instrument alone to monitor particle systems without attention next to the instrument. EasyViewer has build in automated instrument control functions such as autofocusing when particle size changes and autoillumination when brightness of the system changes. EasyViewer provides bride images over the whole process. Particle size distributions or particle size trends are generated at the same time when measurement goes on.

New React-Raman 802L has designed to reach next level of reliability and sensitivity in in-situ polymorphy and reaction analysis studies. The new design of React-Raman 802L ensures optimized in-situ Raman spectra monitoring with best in class performance, extended reaction analysis software and the small size to fit into every fume hood. Additionally automated parameter settings, extended safety levels and data evaluation with scatter and baseline corrections make the system unbeatable for in-situ characterization environment.

EXPLORING NOVEL CONNECTIONS BETWEEN RAMAN SPECTROSCOPY, MICROWAVE REACTORS, AND RHEOMETERS

Rapta M.

Anton Paar Czech Republic

Chemists face numerous challenges when monitoring reactions, including identifying products and intermediates, optimizing reaction parameters, and detecting intermediates. Our new solution for reaction monitoring, the Raman spectrometer Cora 5001, offers a unique tool for real-time monitoring of chemical reactions. This technology can monitor reactions in microwave reactors, providing a powerful tool for optimizing reactions by linking reaction parameters such as temperature and pressure to concentrations of educts, intermediates, and products in real-time.

Understanding the molecular changes that occur during the process of understanding the macroscopic visco-elastic properties of samples has become increasingly vital in both academia and industry. By combining a rheometer with a Raman spectrometer, researchers can monitor both molecular and macroscopic visco-elastic changes simultaneously, providing valuable insights for research. With a better understanding of molecular changes, such as crystallinity and formation of new bonds, the optimization of newly developed materials becomes easier. Additionally, the Raman spectrometer can be utilized for other general purposes in the lab beyond monitoring molecular changes.

EFFICIENCY EVOLUTION AND KINETICS IN THE CONTINUOUS SCREENING AND BATCH SIEVING PROCESS

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The quality of the screening/sieving process can be characterised by several indicators. In most cases, it is sufficient when these are known only about the final product, but sometimes, e.g., in process optimization, it may be important to know how these indicators have evolved over time.

The experimental material was dry sand with a median particle size of 135 µm, which was the feed material for both the continuous screening process and the batch sieving process. In the case of the batch process, the key parameter is the sieving time, in the case of the continuous process, the screen length. In the first part, the methodology of the experiments is explained, as it was necessary to figure out, how to analyse the material at different time and length sections. In the second part the evolution of the quality indicators and the kinetics of particle passage are shown. Regarding kinetics, the aim was inter alia to validate the theory of particle passage that the probability of passing an aperture is greater for small particles (except for dust) than for coarse particles. By analysing the undersized material in the sections, the passage trend can be tracked.

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PHYSICAL PROPERTIES OF BLACK LIQUOR BEFORE AND AFTER THE IMPREGNATION TEST OF SPRUCE CHIPS

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Black liquor, which is considered to be a complex aqueous solution, was used to study the impregnation cycle of the alkaline batch process of softwood chips. This solution usually consists of an organic fraction (lignin, polysaccharides, low molecular weight resin compounds) and also an inorganic fraction in the form of dissolved salt ions. The initial value of the effective alkali (EA) concentration of the black liquor decreases with time. These curves are time-dependent due to different process parameter settings, whether pressure or temperature. However, a standard indicator is a fact that during the first 10 minutes, this proportion is most pronounced. A decrease in the EA concentration value is associated with a change in the viscosity itself.

The viscosity of the penetrating liquid is considered to be one of the main factors influencing the flow of liquid through the wood structure. In addition to the process temperature at which the impregnation is carried out, it also depends on the amount of solid particles, i.e. the dry solids. It is noticeable from the evaluation that while the black liquor concentration decreased significantly with time, the samples taken after impregnation showed very similar dynamic viscosity values to the original solution at the beginning of the impregnation.

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ENHANCED DRYING – HEAT-PUMPS, MOISTURE MONITORING, DRYING KINETICS

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Industrial drying is an energy-intensive process due to the high energy input required for water evaporation. Conventional industrial air-drying uses fossil fuels to heat the air that dries the products. The exhaust air, which is not dry enough for a new drying process, still contains useful heat that can be recovered by a heat pump. This environmentally sustainable solution reduces the dependence on fossil fuels, provides significant economic savings - especially given the recent increase in energy prices – and mitigates CO2-emissions. Yet, the integration of a heat pump requires a re-evaluation of the temperature levels that affect drying conditions and product moisture content, which can be monitored and result in an additional energy savings by eliminating the need to over-dry products. It is also necessary to study the effects of altered drying conditions in the laboratory before applying them directly in the industrial dryer. The drying kinetics of the products in question should be determined with a measuring device that can establish the temperature, humidity, and velocity profile of the air in the laboratory drying chamber. This contribution introduces enhanced industrial drying by presenting a concept for heat pump integration, a concept and device for product moisture measurement, and mainly, a newly developed prototype laboratory dryer for continuous study of drying kinetics of large samples. This work was carried out as part of the EDDY – Enhanced Drying, FFG project number 880778. EDDY is a subproject of NEFI – New Energy for Industry, a flagship region funded by the Climate and Energy Funds Austria.

MONITORING OF PYROLYSIS ENVIRONMENT DURING CORROSION TEST WITH WEDM MACHINED STAINLESS STEELS

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Pyrolysis represents one of the most convenient technologies for the chemical transformation of waste. The exposure to corrosion products and high temperatures does, however, require chemically resistant construction materials. This study was carried out to analyse the corrosion behaviour of 1.4571 (AISI 316Ti) and 1.4305 (AISI 303) stainless steels machined with wire electric discharge machining (WEDM) in a pyrolysis environment.

The corrosion resistance was tested in a modified batch pyrolysis unit. The pyrolysis took place in the furnace at 500 °C with wood chips as the feedstock. The products were carried by a nitrogen via heated paths to a test furnace where the test pieces were suspended. The total testing time was 28 days, with the test furnace refilled 12 times. The samples of the gaseous products were taken from the apparatus outlet in order to characterize the environment where the tested steals were positioned. The condensed gases analysis was done with gas chromatography–mass spectrometry.

The change in the composition of oxygen-containing substances (acids, alcohols, ketones) and aliphatic hydrocarbons (alkanes, alkenes) showed significant changes. The furans and aromatic compounds, for instance, benzene, naphthalene, and its derivatives, were the only substances identified from the higher hydrocarbons. Many PAHs, such as phenanthrene, anthracene, fluoranthene, and others, were identified as well. The secondary reaction mechanisms greatly influenced the content of the pyrolysis products due to their prolonged stay in the setup. This was also connected to the formation of C–C bonds and carbonaceous deposits on the surface of the test furnace and metallic samples.

30 YEARS OF HYDROPROCESSING AT UCT PRAGUE: THE TRANSITION FROM PETROLEUM FEEDSTOCKS TO BIO-OILS FROM HTL AND PYROLYSIS

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Hydroprocessing including hydrotreating and hydrocracking is a key refinery process commonly used for the upgrading of various petroleum fractions to produce transportation fuels or feedstocks for other processes. Our Department of Petroleum Technology and Alternative Fuels at the University of Chemistry and Technology, Prague investigates hydroprocessing for more than 30 years. We started with the hydrotreating (mainly HDS) of petroleum middle distillates and successfully solved all challenges connected with decreasing the limits of sulfur content in diesel fuel. The transition to biofeedstocks started more than 15 years ago when we focused on vegetable oils and animal fats HDO to hydrocarbon-based fuels. It is more than 7 years since we had to push our abilities to a new level starting with the study of hydrotreating (mostly HDO) of bio-based feedstocks like bio-oils derived from the ablative pyrolysis of straw or miscanthus. It is almost two years since we started a collaboration with Aarhus university and deal with the upgrading of HTL biocrudes derived from cow manure and straw. Since that time, we processed by hydrotreatment HTL biocrudes from various feedstocks like waste cotton and textile, water treatment sludge and pyrolysis oils from waste tires and plastics. We cooperate on this research with several refineries like Crossbridge Energy, BayernOil and Orlen Unipetrol. As each feedstock differs significantly, we had to make a corresponding modification of the catalytic unit. In the meantime we built the unit for the hydrocracking of liquid samples and samples which are solid at room temperature. The unit is equipped with a 6-heating zones furnace and 14 thermocouples in a catalyst bed for the perfect temperature control and monitoring. The unit was used e.g. for the hydrocracking of Fischer-Tropsch wax with a melting point of around 120 °C, isomerization of durene-based feedstock and hydrotreating of biocrudes derived from water treatment sludge.

MATERIALS ENGINEERING

MICROSTRUCTURE OF ALUMINUM SINGLE CRYSTAL AFTER COMPLEX SEVERE PLASTIC DEFORMATION

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The complex way of severe plastic deformation which produces thin-walled tube from a solid rod – complex shearing of extruded tube – was applied to an aluminum single crystal. Thie procedure involves extrusion of a solid rod followed by two ECAP-like processes. Additionally, a shearing of the inner surface of the originated tube may be realized by rotating mandrel. It is shown that in this one-way-process, an ultra-fine-grained microstructure is obtained even from the starting single crystal of aluminum at room temperature. Individual steps of the process are characterized not only by the changes of the microstructure but also by changes of the preferred orientations. The effect of the shearing of the inner surface of the tube during the process is also discussed.

NON-CONVENTIONAL APPLICATIONS OF INTERMETALLICS

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Intermetallic compounds are very interesting materials, having the properties between metals and ceramics. Due to this fact, they enable e.g. utilization at high temperatures or in severe corrosion environments. Many intermetallic compounds also have other functional properties, such as shape memory effect. Due to these properties, intermetallics are promising materials for application in automotive or aerospace industry. Most of the industrially important intermetallics (aluminides, silicides and Ni-Ti alloys) are CRM (critical raw materials) – free or low–CRM. This paper summarizes current applications of intermetallics, possible future trends in this industrial branch and new solutions developed by the authors. The proposed future applications of intermetallics are especially in tooling industry. The advantages and problems of the new approaches are discussed individually.

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THE INFLUENCE OF ALLOYING ELEMENTS DISTRIBUTION ON DEGRADATION BEHAVIOUR OF TIN-RICH MATERIALS

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Tin-rich alloys degradation may happened by change of modification from white tin to grey tin, also known as a tin pest. The influence of individual alloying elements has not been reliably described, yet. The most common alloying elements present in historical organ-pipes are Pb, Cu and Fe. It has been stated that Pb suppress the tin pest even in low concentrations. In our work, we focus not only on the concentration of the alloying element but also on the distribution, which is usually neglected. In dependence on heat-treatment, the Pb can be in the Sn matrix present in thee forms: i) as large particle after casting, ii) as solid solution after homogenization annealing and iii) as fine precipitates after ageing. The transformation behaviour of these the states of the model alloy with 0.8 wt. % of Pb was studied.

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EASILY TUNABLE PROPERTIES OF HIGH-ENTROPY CANTOR ALLOY BY CHANGING ITS COMPOSITION

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Since 2004, materials research, especially the commonly chosen preparation strategy got a new impulse deflecting from the centuries-proven approach. The main alloying element became insignificant since the newly announced branch of High-entropy alloys (HEAs), was thought to be based on the equiatomic proportions of each element, having high configurational entropy. This, together with at least five or more elements, stabilizes the disordered solid solutions within the microstructure and is considered one of the four core effects. More importantly, having a large amount of randomly distributed atoms creates a lattice distortion lowering in total perspective the diffusion speed of elements within the alloys, both known as another two core effects. The cocktail effect stating the existence of the synergic contribution of each element to the overall performance of the alloy, is known as the last fourth effect, being mentioned regarding the HEAs. As the research of the HEAs continued, the initially announced rigid borders became loose, re-defining the content of each alloying element to ranging from 5 to 35 at.% or even allowing the HEAs to be composed of other phases instead of solid solutions. Nevertheless, the HEAs are opening a brand-new group of materials that comprise high strengths while retaining their ductility. More importantly, these results are accompanied by good corrosion resistance, showing also good thermal stability. As it was discovered, a change in one of five elements in the most pronounced Cantors alloy is capable to deliver completely new and surprising results, which are further tunable by the content of this element. Therefore, the properties of these alloys are controlled not only by changing the sole element itself but also by its actual content within the alloy, opening an easy way to deliver materials with tailored properties.

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MICROSTRUCTURE AND PROPERTIES OF THE REFRACTORY HIGH ENTROPY ALLOYS

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Refractory high entropy alloys are advanced materials, which are composed of 5 or more elements with high melting temperatures. Due to their high configurational entropy, their microstructure is composed of solid solutions enabling them to achieve extraordinary properties. Refractory high entropy alloys based on MoNbTaVW are characterized by good mechanical properties, which are retained even at elevated temperatures. However, the high-temperature oxidation of these alloys generally limits their applicability. In the frame of this work, the oxidation resistance was improved using the substitution of W and V by Ti and Al. 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.

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MIKROSTRUKTURA A VLASTNOSTI ŽÁRUPEVNÝCH SLITIN S VYSOKOU ENTROPIÍ

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Žárupevné slitiny s vysokou entropií jsou pokročilými materiály, které jsou tvořeny z 5 a více prvků s vysokou teplotou tání. Díky jejich vysoké entropii je jejich mikrostruktura tvořena tuhými roztoky, díky čemuž dosahují výjimečných vlastností. Žárupevné vysoko-entropické slitiny tvořené prvky MoNbTaVW se vyznačují velmi dobrými mechanickými vlastnostmi, které zůstávají zachovány i při vysokých teplotách. Z hlediska odolnosti vůči vysokoteplotní oxidaci jsou však vlastnosti těchto slitin nedostatečné pro jejich budoucí aplikaci. Cílem této práce bylo zlepšení oxidačních vlastností pomocí substituce W a V za Ti a Al. U připravených slitin byla pozorována mikrostruktura a jejich fázové složení a byly měřeny jejich mechanické vlastnosti. Dále byla popsána vysokoteplotní oxidace a mechanické vlastnosti při zvýšené teplotě.

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INFLUENCE OF MN AND AL ON ADVANCED HIGH-ENTROPY ALLOYS PREPARED BY MECHANICAL ALLOYING

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High-entropy alloys (HEAs) have recently emerged as materials that changed our perspective on alloys in general, gaining exponentially increasing attention among the broad scientific community. In contrast with the traditional alloying concept, HEAs are composed of five or more elements, each with a concentration between 5-35 at.%. A rise in configurational entropy, increased by the higher portions of elements typically in near equal amounts, along with other criteria showed a substantial effect on the microstructural composition of these alloys, which might be solely formed of solid solutions, e.g. the CoCrFeNiMn alloy. This alloy constitutes only FCC solid solution exhibiting interesting mechanical properties while maintaining high ductility.

In the presented work, the influence of Mn and Al on the properties of advanced high-entropy alloy, prepared by a specific approach, was examined. The prepared alloy showed superior mechanical properties far exceeding those prepared by more conventional techniques.

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MICRO AND NANOSTRUCTURING OF AMORPHOUS CHALCOGENIDE THIN FILMS

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Amorphous chalcogenides possess a number of unique properties and interesting effects. Mainly due to the large IR transmission window and high refractive index, chalcogenide glasses are attractive materials for optical applications (e.g. waveguides, diffractive elements, microlens arrays, etc.). In comparison with oxide glasses, the chalcogenide glasses possess weaker covalent bonds which result in their lower rigidity and softening temperatures. Many of them, especially in a thin film form, are sensitive to different types of radiation (such as UV-VIS, electron beam, ion flux ….) often leading to changes in their optical properties and/or their chemical resistance to wet and/or dry etching. Exposure to a focused laser beam or hot embossing can result in direct surface structuring. All these properties predetermine chalcogenide glasses for fabrication of the optical elements operating in IR spectral region and also allow usage of chalcogenide glass thin films as photo- or e-beam high resolution resists for lithography.
Herein, we report the results of 3D micro- and nanostructuring of chalcogenide glass thin films using photo- and electron beam lithography (with subsequent selective etching), hot embossing and direct laser writing. We compare possibilities of structuring of As and Ge based glasses prepared by “classical” vacuum thermal evaporation technique with those prepared by solution-based deposition methods. We have been intensively investigating possibilities of solution-based deposition methods as it gives the opportunity to alter the thin film in composition by adding either a pure element or even by mixing multiple glass solutions. We also demonstrate the possibility to modify the structure/properties of final thin films by adding new components into chalcogenide glass solution (e.g. quantum dots, metal) which can add new functionalities to the structured thin films. Examples of high-quality diffractive optical elements fabricated in chalcogenide glasses are presented.

Acknowledgments
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COMPREHENSIVE CHARACTERIZATION OF CARBON MATERIALS AS POSSIBLE CATALYTIC SUPPORTS USING XRD, HR-TEM, SEM, N_2 ADSORPTION AND XPS ANALYSIS IN RELATION TO THEIR THERMAL STABILITY IN AIR

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The combination of structural, thermogravimetric, and calorimetric analyses under identical conditions for all carbon nanomaterials showed that the most decisive factor in increasing stability is the stacking of graphene layers with long-range order parallel to each other, increasing the onset oxidation temperature (T_{on}) with the number of graphene layers from 530 °C for graphene to 800 °C for graphite. The unsaturated carbon atoms at the defects and edges and the bending stress in the 3D graphene layers cause that graphene, the 3D non-defective monolayer in fullerenes, and the defective monolayer in zeolite-templated carbon exhibit stability similar to disordered amorphous materials, as well as 3D organised mesoporous materials. All these materials are oxidised in a narrow T_{on} interval of 485 to 530 °C. The most significant factor for reducing stability is the presence of specific oxygen-containing functional groups, which decrease T_{on} for materials with oxidized edges and with predominant hydroxyl groups by up to 150 °C. The stability of the analysed carbon materials increased in the following order: GtO < Ox-2LG ~ Ox-SWNTs ~ Ox-GNPs < graphene ~ fullerene C_{60} ~ fullerene C_{70} ~ Y-carbon ~ activated carbon ~ 3DOMM ~ CMK-3 < GNPs < graphite [1]. The relationships between the carbon structure and its stability in the air facilitate targeting the nanostructure of carbon materials for catalysis in relation to their stability.

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INVESTIGATION OF THE STRUCTURE OF TIN ALLOYS IN HISTORICAL ORGAN PIPES BY TRANSMISSION ELECTRON MICROSCOPY

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In this work, samples of historic tin organ pipes were prepared for transmission electron microscopy. The samples were prepared using a precision ion polishing system (PIPS). The aim was to determine the presence and distribution of the phases present. The findings will be used to model degradation processes such as mainly the mechanism of tin plague but also to investigate the corrosion behaviour of these alloys.

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ECONOMICALLY AVAILABLE MAGNESIUM ALLOYS WITH HIGH RESISTANCE TO IGNITION

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This work focuses on the development of a magnesium alloy with improved performance suitable for use in the aerospace industry. While magnesium alloys are some of the lightest metal construction materials, their use in aircraft cabins was prohibited due to safety concerns. However, recent advancements have made it possible to modify the properties of these alloys to meet safety requirements. Through alloying, the mechanical, corrosive, and oxidative properties of magnesium alloys are significantly improved. The magnesium alloy presented in this study contains Y, Ca, and Al as the main alloying elements. Selected combination lead to a high ignition temperature, excellent mechanical properties, and an affordable price. The aim of this study is to introduce a light and economically accessible magnesium alloy that meets safety standards and is suitable for use in the aerospace industry.

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ZINC MATERIALS PREPARED BY POWDER METALLURGY

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Zinc has emerged as a promising biomaterial due to its excellent biocompatibility and corrosion resistance. However, its poor mechanical properties and limited bioactivity have posed challenges for its applications. Recent studies have focused on improving the properties of zinc by incorporating other elements, modifying its microstructure, and applying surface treatments through various preparation processes. These approaches have shown promising results in enhancing corrosion resistance and bioactivity. The future of zinc-based biomaterials lies in developing novel alloy compositions with preparation processes that can improve their properties for specific biomedical applications.

Our research focuses on the synthesis of novel, nano-grained zinc materials using powder metallurgy techniques, specifically mechanical alloying (MA), in combination with fast compaction techniques such as spark plasma sintering (SPS). By selecting the correct processing parameters and adding alloying elements like magnesium, we generate a fine microstructure with homogeneously distributed intermetallic phases. Grain refinement with solid solution strengthening significantly enhances mechanical properties. However, oxidic structures from the original powder particles remain in the microstructure, which can increase the likelihood of localized corrosion and brittle cracks. To address this issue, we employed additional thermomechanical processing, specifically extrusion, which broke the oxidic structures into nanoparticles. This, in combination with the newly developed texture, led to even higher improvement in both mechanical and corrosion properties.

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HYDROGEN EMBRITTLEMENT OF 3D PRINTED HIGH STRENGTH 1.2709 STEEL

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Hydrogen embrittlement (HE) is a sensitive problem of all high and ultra-high strength steels, which manifests itself as a huge decrease in the values of mechanical properties and the transition from plastic to brittle behaviour of materials. Hydrogen is a dangerous element because of its small size and high mobility. After it enters a material structure, it recombines from atomic H to a molecular H_2, which is subsequently captured into hydrogen traps and causes changes in a material structure and properties. This can be observed as microscopic cavities, cracks and macroscopic blisters. All these defects lead to destruction of a material integrity. There are two ways how hydrogen can get to a material structure. The first one is a producing method, and the second one is a working environment. Considering that 1.2709 maraging steel is a type of high strength steel, which is widely used in aerospace, military, and energy industries, there is a high probability of hydrogen saturation during the use of maraging steel products. Therefore, it is very important to know maraging steel response to hydrogen saturation (HS). In this study, two types ("as-built" and "as-built + SAT") of a high strength additively manufactured 1.2709 maraging steel were used. The steel was examined for changes in mechanical properties, fracture surface, and the amount of absorbed hydrogen before and after 24 h electrochemical saturation with hydrogen.

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TECHNOLOGY OF DED AS NEW REPAIR PROCESS OF HIGH PRESSURE DIE CASTING

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High pressure die casting moulds are used for casting non-ferrous metal alloys. In automotive operations, they are used in the production of pieces with a complex shape, such as an engine block. The advantages of high-pressure casting are high productivity, high accuracy, and excellent mechanical properties of the casting. Molten metal is cast into moulds that are made of tool steels. The most commonly used steels are AISI H11, which is used due to high mechanical strength even at high temperatures, great toughness, fatigue resistance and dimensional stability.

During casting, the most often occurs the sticking of the metal on the mould. This aspect can change the geometry of the mould. Then the casting process is no longer possible and the mould needs to be repaired. Second commonly viewed problem is the cyclic thermal-mechanical loading of the moulds, which leads to cracking of the surface of the shapes on sliders.

Conventional methods are commonly used for the repair of high pressure die casting moulds. Mould repair consists of milling the damaged area, welding a new shape and milling it to the final size. In order to maintain the same properties of the welded part and the base material, the base material is preheated and then heat treated. Due to the fact that the welded shapes can have a complex geometry, it is difficult to achieve an ideal weld by manual welding. A different amount of material is welded during each repair. All the mentioned aspects make the process longer. With the DED (Direct Energy Deposition) technology, it is possible to speed up the entire repair process while also improving the mechanical properties compared to other repair techniques. In this work, the mechanical properties, structure and heat treatment of the conventionally processed material 1.2343 (AISI H11) and the material Ferro 55, which was prepared by DED technologies, are compared. This work also compares the properties of the Ferro 55 material processed by DED technology with the properties of the same material processed by SPS (spark plasma sintering) technology, when this method of metal preparation results in minimal porosity and minimal thermal influence and thus the gain of maximum mechanical properties.

3D PRINTED TI-NI ALLOYS PREPARED BY SELECTIVE LASER MELTING FOR SOLID-STATE COOLING TECHNOLOGIES

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Currently, shape memory alloys (SMAs), including NiTi-based alloys, are among the widely considered materials for developing alternatives to vapor compression HVAC technology. The aim of the present work is to study equiatomic NiTi elastocaloric materials prepared by 3D printing technology specifically Selective Laser Melting /SLM/ using pulsed and continuous mode.

The 1 cm^3 samples were characterized with differential scanning calorimetry, X-ray diffraction, electron microscopy including back-reflected electron diffraction and mechanical loading in compression. The porosity of the samples was from 1 to 20 % in dependence of the parameters of the SLM method. In terms of microstructure, the samples did not show preferential grain orientation in the direction of building or in the direction normal to building. The grain size ranged from 10 to 500 µm. Latent heat values range from 20 to 30 J/g.

VINTAGE HARLEY-DAVIDSON MOTORCYCLE VALVE STEEL STRUCTURE STUDY

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The study is focused on poppet valves as an important part of combustion engines. Tightness of a combustion chamber is one of elementary parameters impacting exhaust emissions as well as life of the whole engine and other parameters during operation. Next serious issue of combustion engine valves is a complete failure with consequent vast damage of a cylinder, piston and cylinder head. Aim of the study is to compare internal material structure of heavily used exhaust valves with their unused equivalents to reveal degradation mechanisms. Concerned machine is Harley-Davidson WLC 1942 motorcycle fitted by V-twin 45'' flathead engine, equipped by four valves, originally using 72 octane leaded petrol. For the characterization of martensitic valve steel X45CrSi9-3, following techniques were used: macrophotography, light optical microscopy, Electron BackScatter Diffraction (EBSD), Electron Channeling Contrast Imaging (ECCI) and micro hardness profile testing.

The contribution is a part of larger project which considers that despite planned replacing combustion drive units by electrical ones in following years, there are several important branches, where this change is found to be difficult to happen. Cargo transport trucks, ocean ships, construction equipment, agricultural machinery, emergency & battle vehicles cannot be powered by electromotors so far without a significant technical progress on vehicle accumulators. Very recent classical combustion engine alternative that employs past 150 years of thermal drive units research & development lies in hydrogen-combusting engines. Examination of heat resistant steels, as commonly used material in automotive industry, aged in service conditions for a very long time can be very important for the design of hydrogen-combusting motor components designed to work for long time in a reliable way. Since the EBDS & ECCI analysis techniques are widely known in research area, they are significantly less employed in the industry so far.

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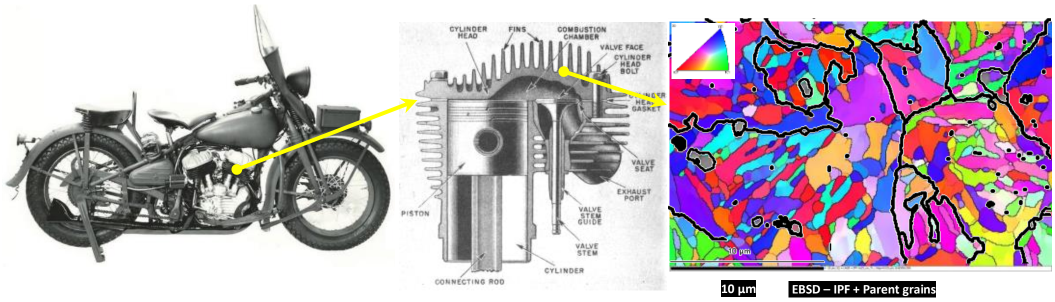

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REDUCED DEEP-SEA NODULES AS AN ADDITIVE FOR ALUMINUM ALLOYS

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Deep-sea nodules represent a scientifically interesting source of valuable metals (Cu, Ni, Ti, Co) but for a long time will surrender to already developed deposits above sea level in terms of profitability. At the current stage of technological development, we cannot influence the cost estimate of mining, but we can design more simplified methods of subsequent processing. Will the resulting product have application value?
In our study, the primary product of nodule aluminothermic reduction, a manganese-based alloy, was proposed as a natural alloying additive for aluminum. For the comparative analysis, we chose the commercial cast AlMn10 master alloy. After a set of modern powder metallurgy operations: rapid solidification by Melt-Spinning, cryogenic milling and Spark Plasma Sintering (SPS), microstructure, mechanical and tribological properties were investigated in order to identify the positive and negative effects of our polymetallic additive. In bending test, new aluminum alloys have showed higher values of flexural ultimate strength compared to commercial referent. They did not surpassed according to other scores, but nodules` mixture showed potential in use as an additive, improving the properties of pure aluminum to a level close to the conventional alloys of 3xxx group.

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RESISTOMETRIC METHOD FOR CORROSION MONITORING

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Most metallic materials are exposed to atmospheric conditions, where their corrosion occurs. Corrosion monitoring techniques are used to gather information about corrosion processes which leads to preventing or at least minimizing damages caused by corrosion processes. A principle of resistometric method and development of this technique will be discussed.

The development of resistometric method consisted of surface treatments of the sensors. Real metallic materials appear in different states of surface such as: polished, coated, corroded, etc. Therefore, there is an effort to prepare sensors with a surface relatively like a surface of real metallic object. The corrosion response of surface treated sensors was observed. Chosen surface treatments for experiments were: polished surface, etched surface in H_3PO_4 or HCl, precorroded and passivated surface. The process of precorrosion was carried out by an exposure to an aggressive environment or prolonged exposure to the outdoor atmosphere. The sensors we worked with were steel and zinc with different shapes and thicknesses of metal traces. The sensors were exposed to corrosive environments to see differences in responses after surface treatments.

It is better to measure corrosion rates on surface treated sensors because the results obtained are closer to the actual corrosion rates than on untreated sensors.

SURFACE TREATED TITANIUM ALLOY FOR PROTON EXCHANGE MEMBRANE FUEL CELLS BIPOLAR PLATES

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Proton Exchange membrane fuel cell (PEMFC) is a promising alternative to combustion engines. It should not compete with battery electric vehicles, since both are suited for a different type of transport. Batteries are a good solution for short distances, cities and light duty. PEMFC, on the other hand is more suitable for heavy duty and longer distances. Advantages of PEMFCs over engines are lower emissions, low operating temperature, low noise and higher energy efficiency. Main disadvantage is the high initial cost of PEMFC, where up to 40 % is the price of bipolar plates.

Bipolar plates serve several important functions, gas distribution, current collection, mechanical support, water management and others. High demands are required in terms of electrical and thermal conductivity, mechanical and corrosion properties, gas impermeability and hydrophobicity.

Currently produced bipolar plates for stationary usage are made of graphite, which is too brittle, bulky and heavy for automotive applications. Where coated stainless steel and titanium bipolar plates are taking their place. The coatings are mostly gold and platinum based, making bipolar plates more expensive. Therefore, there is a demand to find another suitable material.

Titanium and stainless steels with high Cr, Ni and Mo content show good corrosion properties. Current densities are close to the targets set by US Department of Energy (DOE), although at higher potentials (0.6 V/ACLE) they exceed the 1 $\mu A \cdot cm^{-2}$ by double at max. The main issue is interfacial contact resistance (ICR), which is far from the limit 10 $m\Omega \cdot cm^2$ for any material. For titanium and Titanium Grade 7, the ICR is greater than 1200 $m\Omega \cdot cm^2$ after long-term potentiostatic test. With a proper surface treatment, Titanium Grade 7 can be enriched with Pd and its ICR decreases 4 times. Despite the high ICR value, its performance in the in-situ fuel cell test improves significantly.

PREPARATION OF TITANIUM ALUMINIDES-BASED COATINGS USING POWDER METALLURGY

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Titanium and its alloys are widely used materials especially in aerospace due to their favourable strength to density ratio. They also excel in oxidation resistance due to the formation of a passive TiO_2 layer. However, this layer fails at temperatures above 600 °C and titanium needs to be protected in other ways. In this work, several possible approaches to prepare high temperature aluminides coatings for titanium materials using powder metallurgy are discussed: 1) mechanical alloying to prepare aluminide powders in combination with SPS compaction, 2) reactive sintering to prepare aluminide powders in combination with SPS compaction, 3) reactive sintering between powdered aluminium and a compact titanium substrate for one-step synthesis to create an intermetallic coating. All these methods led to the formation of a coating consisting mainly of titanium aluminides on a titanium substrate, and using X-ray diffraction, predominantly intermetallic phases γ-TiAl and $TiAl_3$ were found. The coatings were further compared based on their microstructure, mechanical properties and resistance to high temperature oxidation.

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NEW MATERIALS FOR H_2, CO_2 CAPTURING

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Carbon dioxide (CO_2) is one of the main greenhouse gases that has contributed significantly to global warming in the last few decades. To cope with rising CO_2 emissions, CO_2 capture by specially designed porous and functionalized nanomaterials is one of the promising solutions to reduce the concentration of this gas in the atmosphere.

Adsorption of CO_2 by solid-state adsorbents is considered to be one of the methods offering good reusability compared to aqueous amine absorbent systems. Several materials with different morphologies and functions, such as metallic organic frameworks (MOF), zeolites, organic-inorganic hybrids, metal oxides, graphene, functionalized silica, activated carbons or polyaniline-based adsorbents have been described and studied for CO_2 capture.

We developed several new materials for CO_2 capturing based e.g. on (i) polyaniline/aramid nanocomposite[1] or (ii) mixed matrix membranes (MMMs)[2]. These types of membranes combine the advantages of two main components, both the polymer continuous phase and the nanoparticle dispersion phase. We present new MMM composed from PEBA membrane filled with 2 different amino- compounds of variable concentrations for CO_2 capturing. Different concentrations of amine compounds were chosen to achieve an optimal PEBA membrane structure that would be stable and suitable for further experiments.

Similar approaches now we use for development of materials for H_2 capturing.

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OBSERVATION OF THE MASS TRANSFER ZONE DURING VOC ADSORPTION

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Mass transfer zone observation, during adsorption, in a column is possible by breakthrough curve determination. In many cases, adsorption has an exothermic effect and the mass transfer zone could be determined by temperature (directly in the column by thermocouples). In our research, we observed, that the exothermic effect of ethanol during adsorption onto granulated activated (GAC) carbon is significant. We observed that local increase of temperature during ethanol adsorption can reach temperatures up to 60 °C (adsorption at laboratory condition, 25 °C). The level of temperature increase depends on ethanol concentration in the gas phase during adsorption. All experiments take a place in our newly developed patented device for VOC separation. Our device works on the principle of four processes: stripping, adsorption, desorption, and condensation. In our research, we proved, that it is possible to determine the mass transfer zone, during the adsorption of ethanol, by temperature.

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EKOTOXICITA A BIODEGRADACE LEPIDLA NA BÁZI IZOKYANÁTU

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V oblasti lepidel určených pro nosné dřevěné prvky je v současnosti prioritou používat lepidla s co nejnižším dopadem na životní prostředí, která současně neobsahují formaldehyd. Jednou z možností je použití polyuretanového lepidla. Lepidla jsou však obecně materiály, u kterých se prakticky velice špatně hodnotí ekotoxicita či biodegradace a environmentální hodnocení u nich většinou bývá založeno pouze na teoretických výpočtech založených na posouzení toxicity jednotlivých látek obsažených v lepidle. Cílem této práce proto bylo otestovat ekotoxicitu/biodegradaci vybraného lepidla po jeho vytvrzení (Lignofix D4, STACHEMA CZ) prakticky, a to na řasách (*Desmodesmus subspicatus*) a kvasinkách (*Saccharomyces cerevisae*). Byla hodnocena biomasa řas a kvasinek v akvatických testech toxicity na připraveném výluhu z lepidla a kultivačním roztoku obsahujícím testovaný vzorek lepidla. Výsledky naznačily různou toxicitu lepidla pro řasy i kvasinky v závislosti na tom, zda byl testován výluh či přímo lepidlo v kultivačním roztoku.

BIOAKUMULACE ZINKU Z ODPADNÍCH PNEUMATIK PRO VÝROBU GUMOVÉHO RECYKLÁTU – PŘEDBĚŽNÁ STUDIE

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Odpadní pneumatiky z dopravy lze využít k mnoha účelům, včetně výroby materiálů ve stavebnictví. Zajímavou využitelností se zdá být jejich aplikace ve formě granulí do různých povrchových materiálů. Při jejich výrobě nebo používání se z nich však mohou uvolňovat různé organické či anorganické látky. To může vést k ohrožení životního prostředí a člověka. Zinek patří k jednomu z takových nejvýznamnějších potenciálně toxických prvků. Z tohoto důvodu jsme testovali toxicitu a bioakumulaci zinku na žížalách druhu *Eisenia fetida* (30-denní biotest) a na hořčici druhu *Sinapis alba* (4-denní biotest). Výsledky neprokázaly mortalitu u žížal, ale byla zjištěna toxicita pro rostliny ve formě inhibice kořenů. U obou organismů byla potvrzena bioakumulace zinku.

THE COMPARISON OF EPOXIDATIONS OF METHYL ESTERS OF VARIOUS VEGETABLE OILS

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Epoxides are chemical substances with an oxygen atom bonded to two adjacent carbon atoms. They are almost exclusively synthesized from fossil fuels and have a variety of applications, such as (i) lubricants, (ii) personal care products, or (iii) they serve as precursors for synthesis of other chemicals. Therefore, the synthesis of epoxides from renewable sources is highly favourable. Epoxides of methyl esters of various vegetable oils (such as rapeseed, sunflower, carrot, peach, etc.) were prepared using the same reaction conditions and their properties were compared. Various characterisation methods, such as IR-ATR, Raman spectroscopy, determination of iodine value and determination of epoxy value were used. The composition of products was monitored using GC-MS. The epoxidation was accompanied by the decrease of iodine value and by the increase of epoxy value. Furthermore, the signal of double bonds decreased (Raman spectroscopy) and the signal of epoxide bonds increased (IR-ATR). The novelty is the identification of individual epoxides of methyl esters using GC-MS (no standards exist yet). Epoxides from renewable sources will reduce the need for fossil fuels and have many applications.

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VOC OXIDATION ON NICKEL-COBALT OXIDE CATALYSTS PREPARED BY A COMBINATION OF ELECTROCHEMICAL PROCESS AND PLASMA JET SPUTTERING ON STAINLESS STEEL MESH

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Emissions of volatile organic compounds (VOCs) in industrial gases are still a major environmental problem. These pollutants can be removed from the air by catalytic total oxidation to carbon dioxide and water as final products. In addition to relatively expensive catalysts containing noble metals, cheaper transition metal oxides are also used as catalysts in this process. The catalysts are usually in the form of pellets. However, the disadvantage of this form of catalyst is the large effect of internal diffusion of reactants in the pellets and the high pressure-drop across the bed.

Circular stainless steel meshes (composition in wt. % Fe 70, Cr 18, Ni 10, Mn 2, mesh size 0.415 mm, wire diameter 0.22 mm) with outer diameter of 25 mm were used as supports for deposition. The electrochemically deposited Ni and Co metal layer (molar ratio 1:1) was calcined in air (10 h at 1000 °C) to form oxides and another layer of Ni-Co oxides was deposited on the formed oxide layer by hollow cathodic plasma sputtering of Ni, Co in an $Ar+O_2$ oxidizing atmosphere at a pressure of 80 Pa. The SEM, EDX, XRD, XPS, N_2 adsorption and H_2-TPR methods were used to characterize the catalysts. The deep oxidation of ethanol was carried out in a fixed bed reactor (25 mm i.d.) at temperatures ranging from 80 to 400 °C using a temperature ramp of 2.0 °C min^{-1}. The inlet reactant concentration in air was 750 ppm and the GHSV was 20 l g_{cat}^{-1} h^{-1}. The activity of the catalysts was evaluated as i) T_{50} (temperature at which 50% conversion of reactants was achieved) and ii) conversion at 200 °C and iii) specific reaction rates at 200 °C.

The results obtained from testing the prepared Ni-Co oxide catalysts in the oxidation of ethanol showed that the activity varies depending on the preparation procedure. The ethanol conversion in the presence of plasma-prepared catalysts increased with increasing amount of Ni-Co oxides on the meshes, while the electrochemically prepared catalysts were completely inactive regardless of the amount of oxides on the meshes. When a layer of oxides was deposited on the calcined electrochemically deposited Ni and Co metals from the plasma, the activity was higher than that of the plasma-prepared catalysts alone. Whether the higher activity of the combined Ni-Co layer process is due to a higher amount of active components, a larger surface area, a different crystallographic structure or surface morphology is the subject of this presentation.

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EFFECT OF HYDROXYAPATITE POWDER CHARACTERISTICS ON THE COMPACTION PROCESS AND RESULTING TABLET TENSILE STRENGTH AFTER COMPRESSION

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The transformation of powder material into a solid unit is a complex process. The compression process can be affected by various factors such as compression conditions or the properties of the compressed material. These factors affect not only the compression process itself but also the quality of the final product.

This research focuses on the effect of compression pressure on the process of tablet compression and on tablet mechanical strength. The powder used in the experiments was hydroxyapatite (HAP), which is a material used as food additive or for medical purposes. The compression process is described using the Heckel equation and the tensile strength of the tablets was determined using a diametral compression test. To introduce the reader to the issue, the first part of the contribution is devoted to a theoretical introduction. The second part of the contribution is devoted to the description of experimental equipment and work procedure. The last part of the contribution presents the results of the experiment and their evaluation. In dependence of the particle size distribution and morphology of the HAP particles the compression pressure significantly affects the compression process and the mechanical strength of the finalized tablet. A series of experiments demonstrated this effect found for different HAP investigated.

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EXTRUSION AND SPHERONIZATION PROCESS APPLICATION

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Extrusion is a manufacturing process widely used in various industries to produce different types of dosage forms such as tablets, capsules, pellets and films. In the extrusion process, a material, is forced through a die under pressure to produce a continuous product with a specific shape and size. This process allows for precise control of the properties of the final product, such as its size, shape and hardness. In the context of extrusion, microgranulates may refer to small, discrete particles that are produced by cutting or breaking up an extruded material. This can be achieved by additional process – spheronization. Microgranulates offer several advantages over other forms of granules, such as improved flowability, increased surface area, and greater homogeneity. Additionally, micrograngulates can be formulated to have specific properties, such as controlled release or improved solubility, making them an attractive option for many industries.

This paper is focused on the extrusion process where the experimental apparatus is a single-screw extruder with a separate rotor and die drive, where the die is used in the form of a sieve. Experiments with model material carried out in this way can serve for various applications in industry, such as the production of microgranules for use in the pharmaceutical or chemical industry, as well as for the design of equipment for the production of granules from the liquid phase or paste.

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CERAMIC PROTECTION OF ANTI-CORROSION LAYERS OF ORGANOSILANE (GPTES) ON STEEL

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The issue of mechanical strength of bond of steel reinforcement in concrete has several variants. In addition to geometrical factors, the corrosion performance of steels of variable chemical composition in contact with the variable composition of concrete play a significant role. One possible method is the surface protection of steels with coatings of organosilane compounds, which increase the corrosion resistance of reinforcements in both acidic and alkaline environments, but on the other hand may reduce their bond strength. This problem is solved by the formation of a surface ceramic layer by plasma or hot spraying, with sufficient adhesion to the steel surface to increase adhesion due to surface roughening. However, since the ceramic coatings thus prepared are always porous to some extent, they must be impregnated with substances which often meet conflicting mechanical, chemical and economic requirements and the requirements of the OPS. In a particular case, the creation of an intentionally highly porous thin-walled corundum coating and its impregnation with 3-glycidyloxypropyltriethoxysilane (GPTES), the measurement of the strength of the ceramic-metal bond and the ceramic-cement paste bond in the stage before corrosion testing is described. Two variants of coatings with average thicknesses of 120 µm and 230 µm, with porosities of 0.36 vol % and 0.97 vol %, were produced by plasma spraying of F 240 mesh alumina. The free pore volume allowed the impregnation of up to 0.83 mg of silane per 1 cm^2 of surface area. The tear strength of the ceramic coating reached 15 MPa, while the bond strength of the coating to the cementitious sealant CEM I-42.5R (pure Portland cement) was 10 ÷ 20% lower due to the influence of the surface structure on the surface tension of the organosilane used.

NICKEL-COBALT, NICKEL-MANGANESE AND NICKEL-COBALT-MANGANESE MIXED OXIDE CATALYSTS IN TOTAL OXIDATION OF ORGANIC COMPOUNDS

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Emissions of volatile organic compounds (VOC) in industrial gases represent a serious environmental problem. These pollutants can be removed from air applying the catalytic total oxidation to carbon dioxide and water as the final products; this process is markedly energy saving compared to the elimination of VOC by adsorption or thermal combustion. Besides the rather expensive noble metals-containing catalysts, cheaper transition metal oxides are also used as catalysts in this process. In order to investigate the activity of different types of oxides, we prepared Ni-Co, Ni-Mn, and Ni-Co-Mn oxide catalysts and examined the effect of metal cations molar ratio in the catalysts on their physical chemical properties and catalytic performance in the ethanol and toluene total oxidation.

The oxide catalysts were obtained by heating of precursors, prepared by coprecipitation of aqueous solutions containing Ni, Co, and Mn nitrates in various molar ratios; the aqueous solution containing NaOH and Na_2CO_3 was used as precipitation agent. After drying, the products were calcined for 4 h at 500 °C in air. The samples were labelled according to the molar ratios of cations, e.g., NiCoMn311. The catalysts were characterized by AAS, powder XRD, Raman spectroscopy, N_2 adsorption, and H_2-TPR. The catalytic reactions were carried out in a fixed bed reactor (5.0 mm i.d.) from 80 to 400 °C using temperature ramp of 2.0 °C min^{-1}. The inlet reactant concentration in air was 750 ppm and GHSV of 20 l g_{cat}^{-1} h^{-1}. The activity of the catalysts was assessed by the reaction rates of R_{130} (for ethanol) and R_{250} (for toluene) determined at 130 or 250 °C.

In the oxidation of toluene, the activity of the single-component oxide catalysts showed the order Ni (0.22) << Co (3.76) ~ Mn (3.82 mmol g^{-1} h^{-1}). The most active binary catalysts were NiCo14 (4.04) and NiMn11 (4.03 mmol g^{-1} h^{-1}) and the most active ternary catalyst was NiCoMn122 (4.30 mmol g^{-1} h^{-1}) sample. For ethanol oxidation, the order of activity of the catalysts was similar: Ni (0.07) << Co (0.37) < Mn (0.42 mmol g^{-1} h^{-1}). The most active binary catalysts were the NiCo14 (0.51) and NiMn11 (0.52 mmol g^{-1} h^{-1}) and among the set of ternary catalysts, NiCoMn122 catalysts (1.20 mmol g^{-1} h^{-1}) was the most active catalyst. Evidently, combination of three transition metal components (Ni, Co, Mn), in which manganese and cobalt are prevailing, led to the most active catalysts in oxidation of examined volatile organic compounds in air.

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SUBSURFACE CHARACTERIZATION OF LAYERED MATERIALS: PREPARATION OF TEM LAMELLAE BY THE LIFT-OUT FIB-SEM METHOD; CORRELATION OF TEM-EDX AND FIB-SIMS DEPTH PROFILES

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One of the most important applications of a dual-beam focused ion beam scanning electron microscope (FIB-SEM) workstation is preparing samples for in-depth transmission electron microscope (TEM) investigation. Samples must be uniformly thin to enable the beam of electrons to penetrate and could be selected from region-of-interested with micrometre precision. The main points of the work are the preparation of lamellae from various bulk materials by the lift-out FIB-SEM method and the correlation between depth profiles from energy-dispersive X-ray spectroscopy (TEM-EDX) and secondary ion mass spectrometry (FIB-SIMS), which is directly coupled with the FIB-SEM instrument. The lift-out FIB-SEM method was used for lamella preparation from conductive and nonconductive materials. The conductive material were titanium aluminide and nanotubes on Ti-6Al-4V alloy. The non-conductive material was a model historical photograph. Lamella from the model photograph can help clarify the negative effect of cleaning agents during a restoration process. During the first step of lamella preparation, there was tested a formation of protective layer from platinum and tungsten. Advantage of deposition of tungsten as protective layer is a sample protection from platinum contamination in surface region, which complicated determination of other elements such as iridium having similar energy in EDS. For a sample of titanium nanotubes, correlation was performed to determining the depth profile of iridium in the nanotubes.

These case studies show the benefits of combining scanning and transmission electron microscopes for precise in-depth material characterization from region-of-interested, which could be selected with micrometre precision.

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CHARACTERIZATION OF SPARK PLASMA SINTERED β TI-30NB ALLOY

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One of the approaches for the preparation of very fine-grained materials with mechanical properties exceeding those achievable by conventional processes is Spark Plasma Sintering (SPS) method. The combination of high temperature and pressure allows the preparation of materials with almost theoretical densities at temperatures below the melting point of the material in a short time. Due to the difficulty of producing titanium alloys by conventional methods, powder metallurgy processes are a promising alternative.

Beta titanium alloys have gained significant attention in the last few decades due to their remarkable properties such as excellent corrosion resistance, good mechanical properties, better formability, and improved biocompatibility. Compared to the commonly used Ti-6Al-4V alloy (α + β structure), β titanium alloys exhibit significantly lower modulus of elasticity while maintaining strength. This is particularly desirable in the medical field for the manufacture of orthopedic implants, where the difference in the modulus of elasticity between Ti-6Al-4V alloy and bone is a significant problem in long-term applications. Another advantage of β titanium alloys is the presence of only non-toxic alloying elements such as Nb, Ta, Mo, Zr and Sn. The Ti-Nb binary systems and various methods for the preparation of these alloys have been intensively investigated in recent years. Currently, there are only a few studies dealing with the preparation of Ti-Nb alloys by SPS. The aim of this work was to prepare a binary Ti-30Nb alloy using Spark Plasma Sintering and to characterize the alloy both in terms of microstructure and mechanical properties.

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DEGRADATION OF ZINC ALLOYS IN SIMULATED BODY FLUIDS

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Zinc and its alloys are frequently discussed materials in the field of biodegradable biomaterials due to their acceptable biodegradability rate and reasonable biocompatibility. At the same time, these alloys stimulate the formation of new bone tissue, which accelerates the healing process. However, a significant downside is the susceptibility to local corrosion, which can cause zinc to fail to perform its load-bearing function for the entire required healing time. As a result, many studies focus on *in vitro* corrosion tests of zinc-based alloys that are performed in aqueous solutions simulating blood plasma. These tests help us to understand the underlying corrosion mechanisms of these materials in the human environment.

In our research, we investigated the effects of compaction techniques on corrosion behaviour of Zn-1Mg alloy and pure zinc prepared from pure powders. The materials were compacted by spark plasma sintering (SPS) and combination of SPS with extrusion. The solutions used to simulate the human body environment were: minimal essential medium, Leibovitz's medium and Leibovitz's medium with added carbonate anions. All these media were supplemented with 5 % fetal bovine serum for system complexity. During exposure in various media, the degradation processes generally slowed down due to the formation of insoluble corrosion products and inorganic salts on the surfaces. After one week exposure, we observed the samples on a scanning electron microscope. We found that the materials prepared by SPS contained oxide shells, which represented areas of preferential corrosion attack. On the other hand, extruded samples were more resistant to degradation in a solutions due to redistribution of microstructure.

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THE EFFECT OF PROCESSING CONDITIONS ON THE BEHAVIOUR OF ZN-1MG-1SI ALLOY

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Biodegradable implants are developed to repair damaged tissues and dissolve into organism once the tissue is healed. Zinc and its alloys are candidates for biodegradable metallic implants due to their good biocompatibility and suitable corrosion rate. However, its mechanical properties, especially strength, are not sufficient. Therefore, improvements in these properties are desirable and can be achieved either by alloying or by appropriate materials processing.

The objective of our research was to compare the mechanical properties achieved by various processing of Zn-1Mg-1Si. Magnesium was selected as one of the alloying elements due to its enhancing effect on the mechanical properties and biocompatibility of zinc. Silicon was selected as a reinforcement, and for its positive effect on the bioactivity of the prepared alloy. Both alloying elements have minimal solubility in the zinc matrix. Therefore, mechanical alloying (MA), which increases the solubility of alloying elements and improves mechanical properties by solid solution strengthening, was selected as the preparation technique. Spark plasma sintering (SPS) was chosen as the compaction technique to preserve fine-grained homogenous microstructure, and extrusion was chosen to redistribute the brittle oxidic structures that remained from the surfaces of the original powder particles.

The microstructure of the Zn-1Mg-1Si, prepared by the combination of SPS and extrusion, consisted of elongated grains of zinc matrix, homogeneously distributed oxide particles, and hard silicon particles that showed no signs of deformation or refinement when compared to materials prepared by spark plasma sintering alone. The preparation by MA, SPS, and extrusion resulted in enhanced mechanical properties attributable to the presence of intermetallic phases, texture, and redistribution of oxides formed earlier by spark plasma sintering.

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COMPARISON OF INORGANIC BINDERS POROSITY MEASURING METHODS

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There are various methods for determining porosity of inorganic binders but they differ mainly in the extent of determining pore size and connectivity. This work deals with the measurement of porosity using several different methods, among which belong image analysis (IA), mercury intrusion porosimetry (MIP) and air pressure method, i.e. determination of the size of air pores in fresh unhardened binder. A set of samples containing varying content of cement and hydraulic clinker-free binder prepared from FBC ash was prepared. The choice of method led to different porosity results, which were assessed. It was therefore possible to observe how the results are affected by the measurement ranges of the individual methods. Furthermore, the dependence of the porosity on the water to binder ratio was evaluated.

ADVANCED DESIGN OF HIGH-ENTROPY ALLOYS

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High entropy alloys (HEAs) are modern materials, combining in their structure 5 or more elements with contents ranging from 5 up to 35 at.%. High configuration entropy, which is characteristic of these alloys, stabilizes the formation of disordered solid solutions within their structure. The exceptional properties of HEAs are directly dependent on their elemental composition, i.e. the resulting synergy of the constituent elements. The synergistic phenomenon can be further enhanced by targeted intermixing of high entropy alloy powders, increasing the beneficial properties. This work aimed to design and prepare high entropy alloys combining two disordered solid solutions by the means of mechanical alloying/milling and spark plasma sintering. The prepared compacts were investigated to determine their phase composition and mechanical properties.

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ONE-POT SYNTHESIS OF EMISSION TUNABLE NANOSIZED $AgInS_2$-ZnS HETEROSTRUCTURES

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Colloidal semiconductor nanocrystals (NCs) have unique optical properties in that they emit diverse colors in the wavelength ranges of visible and infrared light which makes possible their application in diverse fields such as light-emitting diodes (LEDs), optoelectronics, photovoltaics, gamma, and neutron scintillators production [1, 2]. Ternary NCs containing elements from I-III-VI groups, such as copper or silver ($CuInS_2$, $AgInS_2$), have attracted great interest due to their eco-friendliness, low toxicity, appropriate band-gap energies (1.53 eV and 1.87 eV, respectively) and their long PL lifetimes. However, I-III-VI NCs possess relatively weak PL emission and low PL QY possibly due to the high surface-to-volume ratio of NCs which results in surface defects.

Herein, we report the novel approach to the synthesis of $AgInS_2$-ZnS solid solution nanorods by the effective conjunction of two sulfur sources. The combination of (*Z*)-1-(octadec-9-enyl)-3-phenylthiourea [3] and 1-dodecanethiol in one-pot solvothermal synthesis in different molar ratios leads to the creation of heterostructures with a uniform shape and tunable optical properties. The ratios modification of (Z)-1-(octadec-9-enyl)-3-phenylthiourea and 1-dodecanethiol (DDT) in the synthesis of nanosized $AgInS_2$-ZnS solid solution heterostructures led to an almost linear shift of the composition towards $AgInS_2$, consistent decrease in length, and, with a large excess DDT, to the growth interruption of nanorods. It has been found that with large excesses of DDT, there is a partial displacement of metal carboxylates from the protective shell of nanorods with simultaneous passivation of the surface with sulfur. $AgInS_2$-ZnS solid solution nanorods were easily embedded into the polymer matrix without loss in photoluminescence quantum yield (PL QY up to 61.5 %). Yellow-red emitting highly photoluminescent nanorods have a large Stokes shift, which makes them attractive candidates for the fabrication of hybrid polymer-inorganic scintillators.

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THE EFFECT OF Ag^+ AND Cu^{2+} ADDED TO BIOGLASS® ON RESULTS OF *IN VITRO* TEST

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Monitoring the bioactive behaviour is a crucial part of the comprehensive testing that all biomaterials undergo before they can be used in medical practice. The initial testing is carried out *in vitro* in a simulated body fluid solution that has a composition similar to the inorganic part of the human blood plasma. These tests provide valuable insight into how the material interacts with the environment.

Bioactive glasses are widely used in clinical applications due to their high biocompatibility. During their interactions with body fluids, they can induce the formation of a hydroxyapatite layer on their surface, allowing the implant to bond tightly with the surrounding bone tissue.

This study focuses on the *in vitro* behaviour of bulk bioactive glasses that were modified with Ag^+ and Cu^{2+} ions to grant them antibacterial properties. This modification of the base Bioglass® composition with 1 wt.% of Ag and Cu was chosen because infection in the vicinity of implants is dangerous to the patient and can negatively affect the healing process. Additionally, with increasing bacterial resistance to common antibiotics in the hospital environment, it is necessary to find alternative methods to provide an antibacterial effect.

The ability of apatite forming was tested in SBF under static *in vitro* test, according to the international standard (ISO 23317:2014) for 14 days, and compared against non-modified Bioglass samples. The results were monitored by analysing the pH levels of the leachates and the changes in concentration of Si, Ca^{2+} and $(PO_4)^{3-}$ ions using AAS and UV-VIS spectrometry. The samples themselves were also observed for the formation of new layers using OM, SEM-EDS, and XRD methods.

The results showed that the introduction of metallic ions affected not only the rate of interaction but their presence in Bioglass had a significant impact on the composition of the newly precipitated layers.

THE IMPACT OF FLUORINE SOURCE IN THE SYNTHESIS OF CeF_3 NANOCRYSTAL ON THEIR MORPHOLOGY

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The scientific community has paid great attention to studying nanoscale materials due to their unique properties. Particular attention is given to fluorescent materials based on rare earth elements (REE). Undoped and doped REE nanocrystals (NCs) are widely used in medicine as biomarkers [1], in high-energy physics as a part of hybrid organic-inorganic scintillators [2] and as individual scintillators [3], etc.

The properties of NCs strongly depend on morphology, which depends on the synthesis method. Here we report on the study of a new way to synthesize CeF_3 NCs, based on a selection of different fluorine sources. The NH_4F, NaF, and KF were used as sources of fluorine. The interaction proceeded on the surface of the solid and liquid phases, with sequential nucleation and the growth of NCs. All stages of the synthesis leading to the formation of NCs performed in one flask, *i.e.,* one-pot synthesis. It should be noted that while maintaining the other reaction conditions, the growth of NCs proceeded according to an individual scheme due to the different interactions of cerium oleate with each of the selected fluorides. In the case of using NH_4F as a fluorine source, sphere-shaped NCs with an average size of ≈4 nm were produced. But applying alkali-based fluorine sources resulted in plate-like shaped NCs with an average diameter of ≈10 nm (Na^+ salt) and ≈20 nm (K^+ salt). Different decomposition mechanisms of the taken salts with subsequent ion exchange can explain such contradictory results.

The observed effect of fluorine sources on the size and shape of nanomaterials allows us to predict the synthesis results for a significant class of REE NCs. The outstanding optical properties, good and stable dispersibility of synthesized CeF_3 NCs make them attractive for introducing into complex scintillators as an active fluorescent material and opening many possibilities for REE NCs application.

This work was supported by the project “High-sensitive and low-density materials based on polymeric nanocomposites – NANOMAT” (No. CZ.02.1.01/0.0/0.0/17_048/0007376) and grant LM2023037 from the Ministry of Education, Youth and Sports of the Czech Republic.

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STUDY OF THE ALKALI-SILICA REACTION OF PROCESSED FLY ASH AND BOTTOM ASH

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Development of alkali-silica reaction (ASR) in concretes and mortars is, among others, a possible cause of concrete construction failure. However, there are admixtures which can significantly mitigate ASR. Admixtures with such ability are generally pozzolans, moreover, energy by-products (CCPs) give very good results. This work aims to study the effect of the addition of fly ash (FA) and bottom ash (BA) as well as investigate the influence of CCP particle size on ASR development. The ASR was studied using an accelerated dilatometric test according to ASTM 1260, complemented by an assessment of mechanical properties after immersion of tested samples into 1 M NaOH solution for 28 days. Experiments were performed on hardened samples containing 10 wt.% CCPs in 3 different grinding finenesses and with the addition of glass (size fraction 2–4 mm). Experiments performed on hardened samples with FA and BA indicate their positive effect on ASR elimination. The results showed that higher grinding finenesses of the admixtures resulted in minimal changes in the expansion reactions.

CIRCULATING ECONOMY

TREATMENT OF WASTEWATER CONTAMINATED WITH HALOGENATED AROMATIC CHEMICALS, THE CIRCULAR ECONOMY APPROACH

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The technology of textile dyes production mostly utilizes water as the green and sustainable solvent. On the other hand, the aqueous filtrate produced after common separation of acid dyes (using for example so called salting out process) is heavily polluted with high concentrations dissolved aromatic compounds, often with halogenated anilines, halogenated triazines and/or halogenated phenols and their derivatives. These mentioned often non-biodegradable halogenated aromatic compounds increase chemical oxygen demand (COD) parameter together with parameter adsorbable organically bound halogens (AOX) in polluted water streams.
In the presentation, the application of circular economy principles in the possible utilization of different treatment methods effective for the removal of mentioned halogenated aromatic compounds will be discussed.

ZINC ASH WASTE TRANSFORMATION TO FERTILIZERS - SUITABLE FORM FOR PLANTS

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Zinc is well-known microelement, in a short time essentially needed in fertilizers and food. Zinc is necessary for the human immune system – it works as an activator and stabilizer of many enzymes. Zinc plays the role in biosynthesis of chlorophyl and protein stabilization. Plants take up zinc as Zn^{2+} ions. Zinc is mainly needed by corn, cereal crops, winter rapeseed, hops, poppy, grapevine….

Waste from car bodyshells is processed by remelting of such parts in Slovakia. This process produces waste zinc ash. As a part of the task, we solved the possibility of processing this waste into a form suitable for plants. The composition of waste was analyzed during 2 years from individual campaigns. Individual types of raw materials entering the process were analyzed for a presence of lead. As a part of laboratory research, zinc ash was processed into a form suitable for plants. This product was then added into the fertilizer and the effect on fertilizer properties was monitored. The production was tested in a small scale quarter-operational production before the operational trial itself. 3,3 ton of zinc ash were processed into nitrate form. It was necessary to develop an analytical method to determine the end of the zinc nitrate formation reaction. 1000 ton of such fertilizer was produced at the plant. The impact of zinc introduction into the fertilizer on the production processes at the plant was evaluated. Problems that will need to be solved were identified. The effect of zinc on the produced fertilizer was monitored and this fertilizer was compared with fertilizer without zinc. Part of the fertilizer was stored in the big bags. In order to determine the effect of time on the fertilizer, 2 big bags are taken out and checked at regular intervals.

RECYKLACE ODPADŮ

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Recyklace odpadů má v dnešní době vysokou prioritu ve všech průmyslově vyspělých zemí. Jde o výsledek působení celé řady faktorů najednou. Pokud z odpadu vytvoříme nový zdroj docílíme úspory nákladů a zároveň tím pomáháme životnímu prostředí. Redukujeme množství odpadu, který by byl uložen na skládce nebo jinak zlikvidován. A ještě si tím vytváříme substitut, kterým nahradíme vstupní surovinu. Zejména státy EU se vyznačují vysokou průmyslovou rozvinutostí na straně jedné a nízkými zdroji vstupních surovin na straně druhé. Absence vlastních surovin implikuje potřebu jejich dovozu ze třetích zemí, což je spojeno s přepravními náklady, období covidu navíc přineslo zpřetrhání logistických řetězců a to se projevilo výpadky jejich dodávek a nárůstem jejich cen a ani v současnosti se situace zcela nevrátila do normálu. To je způsobeno i celkovou geopolitickou nestabilitou. Proto zejména EU klade vysoký akcent na aktivity spojené se zpětným využíváním odpadních surovin jako zdrojů pro výrobu všeho druhu v různých odvětví. Což vedle ekonomických a ekologických pozitiv přinese i snížení surovinové závislosti států EU na jiných zemí. Tato základní myšlenka může být nazývána různými termíny jako „oběhové hospodářství“, „cirkulární ekonomika“, „reverzní logistika“ atd.

Např. pokud je znovu použita 1 tuna ocelového šrotu, dosáhne se úspory: 1100 kg železné rudy, 630 kg uhlí, 55 kg vápence a snížení emisí CO_2 o 58 %. Pokud je znovu použita 1 tuna starého papíru, dosáhne se úspory 3,5 m^3 prostoru na skládce, spálením tohoto množství papíru by vzniklo 750 kg emisí CO_2, dále se ušetří 270 litrů ropy, 26 000 litrů vody, 4 000 kWh energie a zachrání se 31 stromů.

Navzdory všem těmto argumentům existuje celá řada důvodů, proč transformace odpadních surovin na vstupní suroviny pro novou výrobu není na mnohem vyšší úrovni.

Cílem našeho článku je popis této problematiky v čase a datech a popularizace cirkulární ekonomiky.

REMOVAL OF CHLORINE DURING PYROLYSIS OF PLASTIC WASTE

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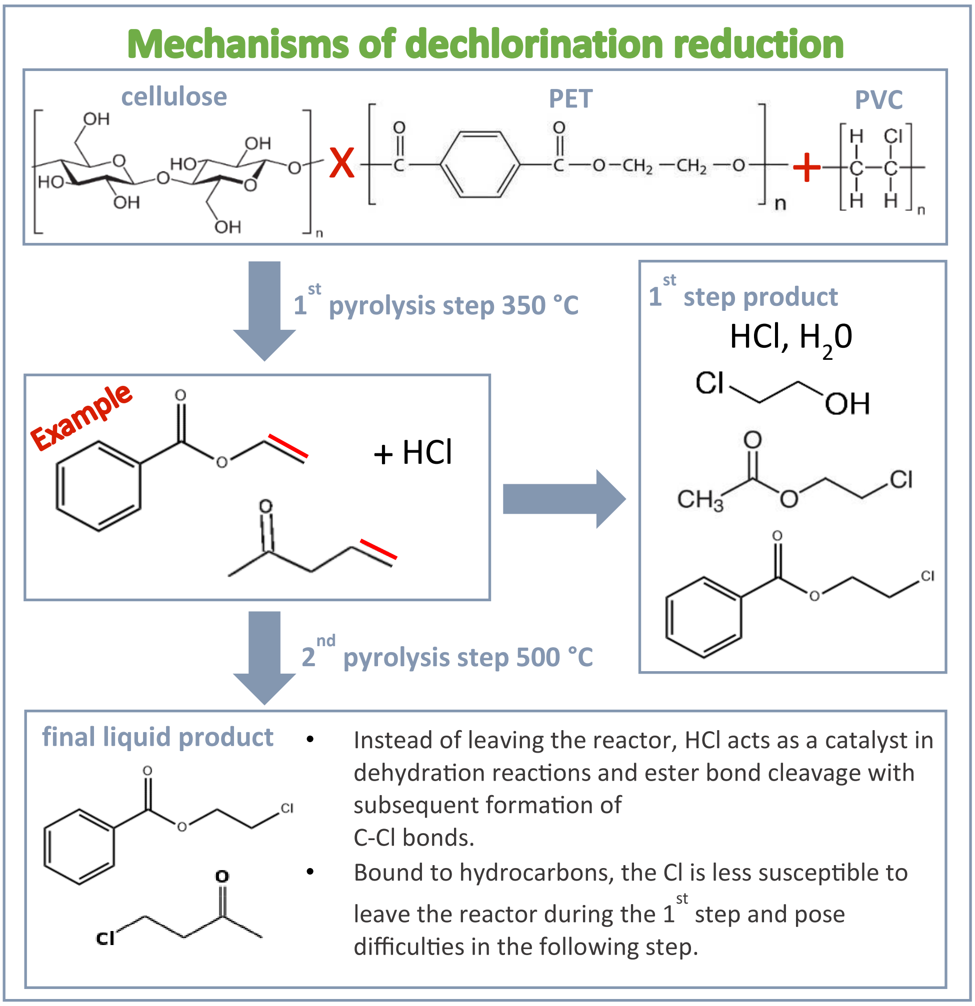
As a complement to mechanical recycling, pyrolysis can be used to recycle complex mixtures of municipal waste plastics (MPW). The subsequent introduction of the liquid product into petrochemical processes can yield virgin polymers. However, there are strict petrochemical limits regarding liquid properties, particularly heteroatom content. In this sense, chlorine is highly inflected because of downstream corrosion and product degradation. The present work, therefore, deals with the possibility of its removal directly in the pyrolysis process. For this purpose, pyrolysis of a model and a real mixture of waste plastics was performed using different temperature programs and dehalogenation agents. The results show a reduced dechlorination efficiency in the pyrolysis of waste plastics, which was subsequently explained by PET and cellulose interactions with HCl that led to the increased formation of more stable chlorinated hydrocarbons. These compounds then pose higher demand on the efficiency of commonly used dechlorination agents. In the present study, we propose a novel mixture of dechlorination agents, which shows a synergistic effect towards dechlorination during MPW pyrolysis based on the interaction of zeolite and hydrotalcite. In combination with stepwise pyrolysis, their presence in 1:1 ratio decreased Cl content in liquid product from 269 ± 34 pmm to 12,2 ± 1,2 ppm. Considering the use of the product as a minor addition to the current technological streams, the achieved dechlorination efficiency may be sufficient.



- Instead of leaving the reactor, HCl acts as a catalyst in dehydration reactions and ester bond cleavage with subsequent formation of C-Cl bonds.
- Bound to hydrocarbons, the Cl is less susceptible to leave the reactor during the 1st step and pose difficulties in the following step.

A PROCESS FOR RECYCLING MIXED TEXTILES CONTAINING PES BY SOLVENT EXTRACTION OF POLYMERS

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Population and economic growth lead to the overproduction of textile materials of different composition and quality. Mixed textile materials consist of two different types, natural and synthetic/polymer fibres, it makes this material difficult to recycle. This work deals with the separation of polymers from two-component textile waste polyester (PES)/cotton by solvent extraction and its effect on the quality of the output recyclates. Dimethylsulfoxide (DMSO) was chosen as a suitable solvent for PES. The solvent extraction was carried out in a glass batch reactor with temperature ranging from 150 - 180 °C and different textile to DMSO ratio. The separation efficiency of the solvent extraction method was controlled by TGA and the effect of the solution on molar mass was measured by GPC. The separation efficiency of the proposed procedure was almost 100%. For recycled polyester, small effect of dissolution on its molar mass was found. Based on the data obtained, the optimum solvent extraction conditions for fabrics with PES were proposed, including the most efficient recycling and purification procedure for the output recyclates.

CHEMICAL RECYCLING OF A MIXTURE OF WASTE LDPE AND PP INTO AN AVIATION FUEL COMPONENT

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Abstrakt

In a conical reactor, cracking was carried out with recycled LDPE and PP waste polyolefins in a 50:50 wt.% ratio at different carrier gas flow rates, polymer feed rates, and reactor temperature profiles. The cracking products are a mixture of hydrogen and C1-C6 hydrocarbons in the gas phase (plus carrier gas), liquid condensate, residual fillers, and carbon. Thermal cracking of LDPE takes place by a radical mechanism with the random splitting of the molecule. This type of cracking results in hydrocarbons with a wide distribution of C1 to C30+ hydrocarbon chains. The cracking of waste polyethylene is dominated by intramolecular hydrogen transfer and β-splitting reactions.

The product of thermal cracking of a 50:50 wt% mixture of waste LDPE and waste PP was rectified on an L=75 cm packed column to a fraction up to 170oC, the aviation kerosene fraction 130-250oC. The kerosene fraction was blended with unsulfurized kerosene from atmospheric distillation of Russian REB crude oil and subjected to hydrotreating refining on a NiMo/Al2O3 hydrotreating catalyst.

The rectified PP cracking product and the blend of PP and LDPE met the requirement of the JET A1 aviation kerosene standard and can be a component of non-sulphur and sustainable aviation fuel components within the circular economy.

Acknowledgements

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COMPOSTING AS AN EFFECTIVE END OF LIFE METHOD FOR BIODEGRADABLE PLASTICS RECOVERY

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Biodegradable plastics occupy more and more trends in the consumer segment. According to the public opinion, employment of biodegradable materials in packaging technology represents a sustainable alternative to oil-based polymers. Indeed, biodegradable polymers such as poly(lactic acid) (PLA) or polyhydroxyalkanoates (PHA) are hot candidates for substitution of so far commercial plastics. Although common consumers put still higher demands on the environmental friendliness of purchased products, the infrastructure for its end-of-life processing is underdeveloped.

Amongst the most aspiring methods of biodegradable waste treatment, composting appears very efficient since releasing carbon from polymer backbone in a nontoxic form and resulting in the formation of a valuable product. Within this aerobic process, complex organic matter is converted into CO_2, H_2O, and biomass. Furthermore, the wide biodiversity of compost provides a rich source of microbes utilizing biodegradable polymers. High temperature reached solely by intensive metabolization contributes to biodegradation progress. Moreover, present additives are possibly bioremediated so leaving no toxic residues. Finally, carbon is ecologically returned to its natural sequestration.

In this study, we have investigated the biodegradation of commercial polyhydroxybutyrate (PHB) and PLA under thermophilic composting conditions. In addition, to evaluate composting applicability at the end of life of biodegradable plastics and, simultaneously, the ecological harmlessness of tested materials, we have further employed final composts in plant-growth supplementation (growth experiments). So far, no negative effects of the compost presence in a substrate were observed. Therefore, we consider this method of recovery of biodegradable plastics as highly potential.

SIMULATION OF OXYGASIFICATION OF PLASTIC FRACTION OF SPENT LITHIUM ION BATTERIES

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With increasing production of electric vehicles and electric gadgets, also the need for their recycling arises, especially of parts like batteries. Lithium ions batteries contain important and valuable materials that can be reused in the production new batteries. In addition to the mentioned materials, several waste streams are generated during battery recycling that are not normally used in the further recycling process. One of these streams is the plastic fraction, which usually ends in landfill. The aim of this study is to show possible use of the plastic fraction as a source in energy valuable syngas production. Syngas can be used as an energetic source or as a source for electricity production, as its consumption during the recycling processes is very high. This gas can also serve like raw material for the production of other substances like methanol, etc. Simulation of syngas production was made in Aspen plus, using gasification with pure oxygen. As a feed material, a mixture of polymeric plastic materials most used in batteries of electric vehicles (mixture of PET, PE, and PP) was chosen. This work also points to the importance and benefits of using multistage oxygasification with recirculation of the final stream compared to simple one stage gasification; the main advantage being lower consumption of oxygen as confirmed by comparison with basic syngas production from the plastic fraction.

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SPOROSARCINA PASTEURII UTILIZING MICROBIALLY INDUCED CALCITE PRECIPITATION FOR THE RECYCLING OF WASTE CONCRETE FINES

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The Paris Climate Agreement, ratified in 2015 by 194 countries, aims to combat global warming and climate change by reducing greenhouse gas emissions, including carbon dioxide (CO_2), among other environmental activities. Cement production, an essential component of the construction sector, is the leading contributor to global anthropogenic CO_2 emissions, responsible for approximately 7 % of the total (Fahimizadeh et al., 2020). To achieve sustainable development and environmental conservation, various strategies have been suggested to decrease energy consumption and CO_2 emissions related to the production of cement. The utilization of hydrated cementitious paste and stripped mortar generated during concrete recycling has been investigated as a potential solution to the challenge of waste concrete fines (WCF) disposal.

In this study, the effectiveness of microbially induced calcite precipitation (MICP) was examined using two types of WCF with variations in their age, grain size distribution, and fineness, generated during the processing of disposed concrete structures. An alkaliphilic urease-active bacterium, *Sporosarcina pasteurii* DSM33, was used for the MICP process, which is capable of precipitation of calcium carbonate crystals under the supplement of urea and calcium ions. The experiment was conducted over four different time intervals (14, 30, 60 and 90 days), during which MICP solution was added to WCF and mixed with *Sporosarcina pasteurii*. After each interval, the composites were dried and underwent a thorough analysis of their physicochemical properties, including cohesiveness, porosity, formation and type of carbonate crystals, and compositional analysis.

Based on our findings, it can be concluded that the utilization of ureolytic bacteria for MICP presents a promising approach for recycling waste concrete fines, resulting in a more efficient and environmental-friendly concrete recycling process.

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ORGANIC TECHNOLOGY

STUDY OF THE PROPERTIES OF THE COBALT CATALYST USED FOR THE HYDROGENATION OF ANILINE TO CYCLOHEXYLAMINE

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This contribution deals with the results of experimental study of the specific properties of the cobalt catalyst Co/$CaCO_3$-Na_2CO_3. The catalyst is applied at process of the industrial hydrogenation of aniline to cyclohexylamine in gaseous phase. This catalyst has very good useful properties as high catalytic activity, selectivity and lifetime longer than 15 years. Specific property of this catalyst is its additional activation called activation period (AP). It is a time period during which, under constant reaction conditions, the conversion of aniline will increase up 2-3 times. This work presents the results of the study of AP and of the others properties of this catalyst, which are summarized, in following bullet points:

- AP is conditioned by the water released and chemisorbed during the reduction of catalyst precursor,
- the water dissolved in aniline results in AP and has promotional effect on the reactivity of hydrogenation of aniline, the highest hydrogenation reactivity is achieved with 1.6-2.0 wt. % of water in aniline,
- it was discovered, that the water modifies the surface of catalyst, leading to partial oxidation of Co^0 actives sites to Co^{2+},
- ammonia eliminates the promotional effect of water on the AP of catalyst and hydrogenation reactivity,
- AP is also conditioned by the chemical promoter Na_2CO_3, other catalysts as Co/$CaCO_3$ and Co/$CaCO_3$-Me_xY_z (Me_xY_z = Li_2CO_3, K_2CO_3, Cs_2CO_3, Na_2SO_4 and $NaNO_3$) show no AP,
- Co/$CaCO_3$-Na_2CO_3 catalyst has low activity for hydrogenation of other aromatic compounds as benzene, toluene, phenylmethanol and *N*-ethylaniline,
- hydrogenation of other aromatic compounds are not affected by the AP of catalyst, with the exception of hydrogenation of phenylmethanol.

PREPARATION OF ESTERS OF TERTIARY ALCOHOLS

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The development of efficient synthetic routes to carboxylic acid esters is of great interest because fine chemicals often contain ester unit as the functional group. The usual methods involve the condensation reaction between an alcohol and a carboxylic acid in the presence of a mineral acid. This synthetic approach results in good yields with primary alcohols, limited yields with secondary alcohols, and poor yields with tertiary ones. The main goal of the work was to find a simple and efficient way for the direct synthesis of esters of tertiary alcohols and to optimize reaction conditions. Dimethylbenzylcarbinol and 1-adamantanol were chosen as model alcohols.

Various synthetic pathways such as Fischer esterification, Steglich esterification, and alcohol acylation with functional derivatives of acetic acid catalyzed by Lewis acids or basic catalysts to obtain esters of tertiary alcohols were tested. It was found that in reactions under conditions of Steglich and Fischer esterification good results were not achieved. In the case of Fischer esterification of acetic acid with dimethylbenzylcarbinol only the undesired product of dehydration 2-methyl-1-phenylprop-2-ene was obtained. Fischer esterification of acetic acid with 1-adamantanol didn’t take place. Although under conditions of Steglich esterification, the desired product was formed, the conversion of alcohols in both cases was only 52-56 % after 24 hours. Acylation with functional derivatives of acetic acid catalyzed by basic catalysts (4-dimethylaminopyridine, triethylamine, pyridine) has given good results (total conversion, selectivity up to 95 %), and no side products were detected in the reaction mixture. Acylation with acetic anhydride catalyzed by hard Lewis acids ($AlCl_3$, $FeCl_3$, $ZnCl_2$) took place with high selectivity (over 99 %) to the desired ester. On the other hand, acylation under the same conditions with acetyl chloride tended to either undesired dehydration of dimethylbenzylcarbinol to give alkene or nucleophilic substitution of a hydroxyl group in 1-adamantanol leading to the formation of 1-chloradamantane. According to the obtained results, we can conclude that acetylation with acetic anhydride in the presence of Lewis acids or 4-dimethylaminopyridine is the optimal way for the synthesis of acetates from tertiary alcohols.

NOVÉ ANTIKOROZNÍ KOLORANTY

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Přednáška se zabývá novou třídou vysoce účinných antikorozních kolorantů, které jsou založeny na solích a komplexech hořečnatého kationu (Mg^{2+}). V přednášce bude i návrh mechanismu antikorozního působení na povrchu železných materiálů.

ORGANIC ELECTROLYTES FOR FLOW BATTERIES

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The advancement of energy production from renewable sources is unthinkable without an efficient electrical energy storage system. In addition to local battery storage facilities, there is great pressure on storage facilities that are directly connected to larger producers, for example in the form of wind or larger solar power plants. In these cases, it is required that these storages are able to maintain energy without loss for weeks or months, and the target requirement is that the price does not exceed 5 €cents/cycle/kWh.
At the same time, the pressure on the use of so-called non-critical materials, i.e. raw materials from non-renewable sources, which are also imported from geopolitically unstable areas, is increasing. Following these requirements, organic red/ox materials are also becoming interesting. They can be used for efficient storage of electrical energy. Organic compounds exhibiting high solubility and long-term chemical stability in water could be suitable for so-called organic flow batteries. It appears as interesting technology mainly for middle period energy storage. Battery is divided into anolyte and catholyte parts and separate storage decrease the risk of self-discharge even after a period of several weeks. A successful solution is based on the correct setting of the electrolytes on the cathode and anode side so that the highest possible potential is achieved. At the same time, it is necessary to complete the overall design of the batteries so that the anolyte and the catholyte can be effectively separated and ensure optimal battery behavior not only in comparison with the vanadium flow batteries already in use today, but also in comparison with lithium batteries.

PRODUCTION OF 4-AMINO-4H-1,2,4-TRIAZOLE AND ITS APPLICATION AS THE NITRIFICATION INHIBITOR.

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The cost effective technology of the 4-amino-4H-1,2,4-triazole preparation has been developed to supply the nitrification inhibitor for the mineral fertilizers.

The inhibitors of the nitrogen nitrification are incorporated into the modern mineral fertilizers to enhance the efficiency of the utilization of this nutrient by plants, reduce the NOx formation and decrease the nitrate leaks into the groundwater. The nitrification inhibitor has therefore favorable economical and ecological effects.

4-amino-4H-1,2,4-triazole is known and efficient nitrification inhibitor. However, its poor availability and high market price present serious obstructions of its utilization in the role of the fertilizer additive. The preparation procedure has been simplified in the laboratories of VUCHT to overcome these drawbacks. Three production steps have been reduced to two. The existing parts of the shut production lines in Duslo have been used to scale up the process. The investment and operating costs are decreased by this way and the product price becomes acceptable for the production of the fertilizers. The cost cuts result in the higher fraction of impurities in the product. It has been necessary to verify that the impurities have no negative impact on the process safety. The fertilizers containing 4-amino-4H-1,2,4-triazole have been subsequently produced and evaluated in the agricultural field tests.

HETEROGENEOUS CATALYSIS OF ETHANOL TRANSFORMATION BY LI-AL MIXED OXIDES DOPED BY TRANSITION METAL

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This work is focused on the transformation of ethanol to more valuable chemical compounds via heterogeneous catalysis in the flow reactor. Ethanol is suitable for this transformation because it can be easily obtained from renewable sources. One of the main products is butanol, which is important chemical compound, because it can be used as solvent or feedstock for production of other chemical compounds, e.g., hexanol, butyl acrylate, iso-butene.

The transformation of ethanol to butanol can be achieved by Guerbet reaction, which is four step cross-condensation of two primary alcohols to the beta-alkylated dimer alcohol. Complexity of the reaction requires catalysis to favor wanted product(s) (butanol), i.e., catalyst can improve ethanol conversion and selectivity to butanol. Metal mixed oxides of lithium, aluminum, and transition metal (Copper) were used as the heterogeneous catalysts for the Guerbet reaction. These metal mixed oxides were chosen as one of the possible alternatives to more common magnesium, aluminum metal mixed oxides. The influence of different amount of transition metal in metal mixed oxides on ethanol transformation was studied and catalytic data were obtained.

The properties of mixed oxides were determined for better understanding of catalytic activity. Namely real molar ratio of metals, crystal structure, specific surface area, reducibility of transition metal and acido-basic properties. Characterization data were statistically analyzed and correlated with catalytic data to determine the most suitable composition of heterogeneous catalysts for the reaction. Addition of transition metal had positive influence on ethanol conversion, on the other hand higher basicity and acidity had positive influence on butanol selectivity. Tuning of heterogeneous catalysts for the Guerbet reaction can provide relatively simple, cheap, and sustainable method of production not only bio-butanol. Because Guerbet reaction has many side reactions, which can be also utilized for production of more chemical compounds. Thus, Guerbet reaction can play important role in sustainable chemistry and gaining independence from strategic resources.

Acknowledgements
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STUDY OF UNCATALYZED LOW TEMPERATURE OXIDATION OF CYCLOHEXYLAMINE WITH AIR IN LIQUID PHASE – EFFECT OF REACTION TEMPERATURE AND CONCENTRATION OF WATER

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Cyclohexylamine is frequently produced by hydrogenation of aniline in gaseous phase over a nickel or cobalt catalysts. During the storage and transport of this amine, its quality can be decreased if there is not excluded contact with air, which leads to arise in concentration of imine *N*-cyclohexylidenecyclohexanamine (NCCHA). It also occurs to the change of the colour of cyclohexylamine from colourless to yellow to faint red. Aim of this contribution is presentation of results of both of the the study of effect of temperature and concentration of water in cyclohexylamine on the reaction rate of its uncatalyzed oxidation with air in liquid phase. The experiments were carried out at reaction temperature 80-110 °C and concentration of water 0.17-1.17 wt. % in cyclohexylamine. From the experimental data the value of activation energy of oxidative dehydrogenation of cyclohexylamine towards NCCHA was calculated, 139.4 kJ mol^{-1}. The used kinetic model consists of the side and consecutive reactions, which accompany title reaction and their kinetic parameters, were calculated. Hydrolysis of NCCHA to cyclohexanone and cylcohexylamine, 89.3 kJ mol^{-1}, condensation of cyclohexanone and cyclohexylamine back to NCCHA, 36.9 kJ mol^{-1} and oxidation of cyclohexylamine to cyclohexanone oxime, 58.5 kJ mol^{-1}. Furthermore, the increasing concentration of water in cyclohexylamine (0.17 wt. % to 1.17 wt. %) has no significant effect on the reaction rate of its oxidation. However, increasing concentration of water 0.17 wt. % to 1.17 wt. % in cyclohexylamine resulted in three times higher reaction rate of the hydrolysis of NCCHA.

HOMOGENEOUSLY CATALYZED ALDOL CONDENSATION OF CAMPHOLENIC ALDEHYDE WITH BUTANAL

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Sandalwood oil finds its application mainly in the perfume industry, where it is still one of the most valuable raw materials. It also has other interesting biological properties that could be used in the pharmaceutical industry, such as its antiviral and chemopreventive effects. However, natural sandalwood oil is expensive and difficult to obtain, so the chemical synthesis of substances with the scent of sandalwood is highly desired in the industry. Among the industrial often used synthetic sandalwood-type oils belong 2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)but-2-enol, which is known under many commercial names such as Levosandol, Bacdanol or Sandranol. Levosandol is produced by selective hydrogenation of 2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)but-2-enal, which is known under the commercial name Levosandal. The mentioned aldehyde can be prepared by aldol condensation of campholenic aldehyde with butanal under basic catalysis. Processes performing this reaction under both homogeneous and heterogeneous catalysis have been described in the literature[1,2].

In this work, attention was paid to the homogeneous base-catalysed aldol condensation of campholenic aldehyde with butanal. The suitable reaction conditions leading to the formation of Levosandal in the highest possible yield were sought. Different reaction conditions were studied, namely the amount and type of homogeneous basic catalyst, the influence of the type of solvent, temperature and ratio of starting substances and the influence of the concentration. Under the selected reaction conditions, the experiment was also carried out on a 20x enlarged scale.

Among the chosen homogeneous basic catalysts, the most active for the aldol condensation of campholenic aldehyde with butanal was a 36 % aqueous solution of NaOH in 40 mol. % relative to campholenic aldehyde. A temperature of 75 °C, *N,N*-dimethylformamide as a solvent and a ratio of campholenic aldehyde to butanal of 1:2 were chosen as the most suitable reaction conditions. Under such conditions, almost 100 % conversion and 90 % selectivity to Levosandal was achieved after 30 minutes of reaction. By-products detected in the reaction mixture were butanal autocondensate, and condensate of Levosandal with butanal.

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SYNTHESIS AND FLUORESCENCE OF PUSH-PULL SUBSTITUTED DIPHENYLAMINO-DIPHENYLDISTYRYLBENZENES.

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In last decades, there has been considerable interest in research on solid-state emitters exhibiting emission in the far red or near-infrared spectral region due to their significant impact on diverse fields of technology. [1] Solid-state fluorescence (SSF) has been studied typically on single crystals, thin layers, or polycrystalline powders. [2] The progress has triggered the creation of novel photoluminescent materials, so that photophysical phenomena, which were of rather academic interest in the past, find now real-world applications, such as single-crystal emission in organic light-emitting diodes, lasing, or optical storage. Understanding of crystal packing modes and intermolecular interactions are challenges of crystal engineering which is crucial for fluorescent properties. [3,4]

Researchers have paid attention to derivatives based on the same building block with fluorescent maxima tuned by a variety of simple substituents. Stilbene and 1,4-distyrylbenzene bear remarkable optical, photochemical and photophysical properties. They have widespread applications in many fields ranging from fine chemistry and materials science to biomedicine. [5] Two novel diphenyl-distyrylbenzenes with triphenylamine donor group were synthesized and studied for their high fluorescence in solution as well as in the solid phase.

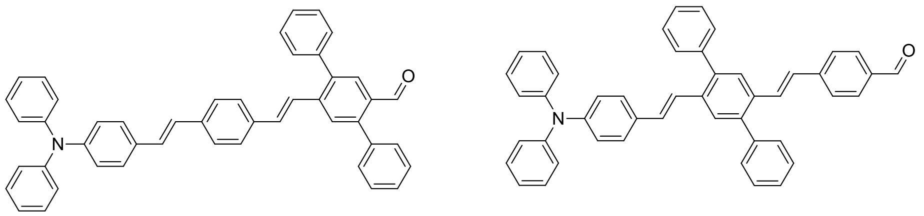

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Figure 1: General structure of diphenylamino-distyrylbenzenes.

Desired molecules were prepared successfully under Horner–Wadsworth–Emmons conditions and after several crystallizations we were able to achieve excellent quality material. The optical behavior was studied in solid state and in various organic solvents by UV/Vis and emission spectroscopy. In conclusion, all prepared compounds promise to be attractive topic for further investigation and application in field of optoelectronic devices.

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ETHERIFICATION OF TETRAHYDROFURFURYL ALCOHOLNOL AND ETHANOL IN THE PRESENCE OF ZEOLITE-BASED CATALYSTS

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In the face of fossil fuels depletion, efforts in developing alternative bio-based fuels and fuel additives are of paramount importance. In this regard, ethyl tetrahydrofurfuryl ether (ETFE) is a promising candidate for diesel fuel additive. Its cetane number is 80-90. The engine tests have proven no adverse effects on the engine operation. Sulphur and particulate content in engine emissions was lower in comparison to standard diesel fuel. However, since the energy content in furanic fuels is lower, the fuel consumption was higher in comparison[1].

Up to date most studies on synthesis of alkyl tetrahydrofurfuryl ethers focus on a reaction pathway consisting of etherification with furfuryl alcohol and subsequent hydrogenation[2]. Hereby we present a one-step gas-phase etherification of ethanol and tetrahydrofurfuryl alcohol (THFA) in the presence of various structure types of zeolites in a flow reactor.

We tested a series of zeolite-based catalysts at varying reaction temperature. All tested zeolites displayed a decline in THFA conversion and ETFE yield at 160 °C, accompanied by heavy coke formation. Out of the tested catalysts, H-ZSM-5 achieved the best results. The best result of 14.0 % ETFE yield and 73.0 % THFA conversion was achieved with Si/Al ratio of 25. Catalyst activity also declined severely after 3rd hour of reaction. Reactivation of the catalyst by calcination however did not have any negative effects of reaction results in subsequent runs.

In conclusion, we successfully synthesized ETFE by a one-step method from ethanol and THFA in the presence of zeolites. The main challenge of this synthesis is the quick deactivation of zeolite catalyst and a need for calcination after a short time of reaction.

Acknowledgement:

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GAS-PHASE SYNTHESIS OF CYCLOPENTYL ETHYL ETHER FROM CYCLOPENTANOL AND ETHANOL

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Unsymmetric ethers are a group of promising alternative chemicals for use as solvents. They have been proven suitable for several routine organic syntheses as well as storage of materials requiring anhydrous conditions. They produce smaller amounts of explosive peroxides over time and are better separable from water-based solutions in comparison to conventionally used etheric solvents[1]. Unsymmetric ethers can be potentially synthesized from renewable biomass-derived alcohols. This type of synthesis only adds to their potentials as novelty green solvents.

Based on our previous results with cyclopentyl methyl ether[2], we hereby present a study of the synthesis of cyclopentyl ethyl ether (CPEE). This synthesis utilizes ethanol, which is a less toxic reagent compared to methanol. We studied the performance of several structure types of zeolite catalyst, as well as the effect of varying technological conditions. We studied the effects of temperature and Si/Al ratio of zeolite catalyst on CPEE selectivity. Experiments with different alcohol chains were also carried out.

From the tested zeolite frameworks, H-ZSM-5 performed with the best results. The rise in reaction temperature up to a point caused an increase of CPEE yield and cyclopentanol conversion. Further increase in temperature resulted in further rise in cyclopentanol conversion, however, cyclopentene yield and coke deposition also increased. With increasing Si/Al ratio of H-ZSM-5 zeolite, both conversion of cyclopentanol and cyclopentene yield steadily. CPEE yield displayed a peak and subsequent decline.

In conclusion, we have successfully synthesized CPEE from non-toxic biomass-derivable alcohols. Gas-phase synthesis of CPEE from biomass-derived cyclopentanol and ethanol in the presence of certain zeolites is a promising method for CPEE preparation.

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SYNTHESIS AND CHARACTERIZATION OF NOVEL D-π-A MOLECULES BASED ON THE SKELETON OF CARBAZOL-DIPHENYLSTILBENE

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Fluorescence is a widely-used physical phenomenon in various applied fields, including biology, biomedicine, and technology. One challenge in the synthesis of organic molecules that exhibit fluorescence is achieving this property in both the solid and liquid phases, particularly in the Near-Infrared Region. Molecules of the Donor- π -Acceptor model are promising representatives of such fluorophores.[1]

Donor-π-acceptor (D-π-A) system is created by a conjugated π-system that links a donor unit and an acceptor component at each end of the molecule, enabling intramolecular charge transfer (ICT), creating the push–pull system[1] and leading to a lower energy molecular orbital (MO)[2]. By combining strong electron donor and acceptor units at each end, these fluorophores can alter their fluorescence properties from ultraviolet-visible (UV-vis) to near-infrared (NIR) [1]. In addition to bioimaging and OLED[3], NIR D-π-A fluorophores are used in dye-sensitized solar cells[4], biosensors[5], and nonlinear optical imaging[6]. The choice of donor or acceptor groups plays a crucial role in the properties of the molecules and affects the emission wavelength and the quantum yield.

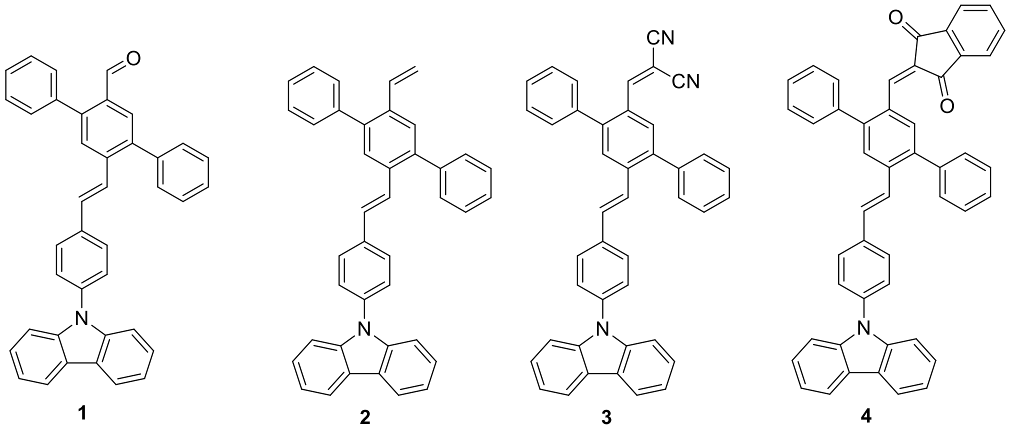

Figure 1: synthesized D-π-A molecules based on the skeleton of carbazole-diphenylstilbene

In this work, fluorescent diphenylstilbene derivatives were synthesized and characterized, carbazole was chosen as a donor and different types of acceptors were tested to see a particular influence on the emission properties of each and to obtain new fluorescent molecules emitting in a solid phase. Different methods and techniques for synthesis were explored, and the most effective ones were identified. The synthesized molecules were also characterized using available methods, and the fluorescence characteristics and possibilities of these new compounds in both the solid and liquid phases were discussed.

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INFLUENCE OF THE REACTION CONDITIONS ON 3-CARENE EPOXIDATION

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Currently, there is an effort to choose a raw material base from a renewable resource. One of the many options is the use of essential oils of plants that are rich on monoterpenes. These compounds are usually fragrant with characteristic scent. Monoterpenes can be oxidized to form a monoterpene oxide (epoxide) that is a simple and selective way to include oxygen atom to the structure. It is possible to carry out various reactions on epoxides, therefore monoterpene oxides are interesting intermediates for isomerizations, reductions, ring opening with a nucleophile, etc. 3-Carene is contained in large quantities in turpentine oil (for example from cypress). Its epoxidation gives 3-carene oxide an important intermediate for the production of, e.g., pharmaceuticals (the reaction of 3-carene oxide with morpholine followed by two other steps gives the second-generation nonnucleoside, reverse transcriptase inhibitor[1]). Conversion of carene and the selectivity to the desired oxide can be affected by oxidant, solvent, catalyst and additives. In the first phase of the study, the synergy of the oxidizer with the solvent was investigated. A decrease in selectivity for 3-carene oxide from nonpolar to highly polar solvents was observed when using *m*-chloroperoxybenzoic acid. This phenomenon can be explained by the solubility of *m*-chlorobenzoic acid as a by-product, which can support the ring opening to form 3,4-carane diol (the undesired product). In the second phase, the influence of the catalyst and additives for the selected oxidizer was tested. Up to now the selectivity 85 % at 97 % conversion was obtained.

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THREE TYPES OF Π-STACKING OF 3,6-DIARYL SUBSTITUTED FURO[3,4-C]FURANONE POLYMORPHS

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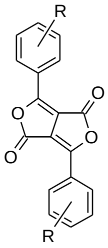
Six 3,6-diaryl substituted furo[3,4-c]furanones (DFF) were synthesized. The computational analysis, based on density functional theory, found eight possible centrosymmetrical slipped π-stack arrangements, formed according to electron repulsion minimization principle. One of these slipped stack arrangements was found to form infinite columns in the crystals by single crystal X-ray diffractometry. All six derivatives show intense solution fluorescence in blue / green region, with a maximum driven entirely by a number and position of methyl substituents on phenyl rings. On the other hand, the solid-state fluorescence from yellow over orange to red is observed only for four derivatives and its presence / absence, spectral position and vibronic structure is driven exclusively by the slips in of π-stacks of almost planar DFF molecules, resulting in J-type emission, H-type excimer-like emission and H-type quenching.



R: H, 2-CH_3, 3-CH_3, 4-CH_3, 2,4-diCH_3, 3,5-diCH_3

Figure 1: Syntheses of the compounds under study.

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CYCLOADDITION OF CO_2 OVER PYRIDINIUM AND IMIDAZOLINIUM BASED CATALYSTS

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The development of efficient organocatalysts for chemical processes is highly demanded in the field of green and sustainable chemistry. Our study presents novel metal-free supported materials based on the salts of *N*-heterocycles. These materials could be used as catalysts for the cycloaddition of carbon dioxide to epoxides. The desired products of the cycloaddition of carbon dioxide to epoxide are cyclic carbonates, which find their application, e.g., as “green” solvents, fine chemical intermediates, and as precursors for the preparation of polymers. Two types of materials were prepared - pyridine and imidazoline based - via impregnation of the molecular sieve MCM-41 by propylhalogen with subsequent quaternization to form the desired salt. The anionic part was represented by bromine and iodine anions. Characterization methods (EA, XRD, TG, UV-Vis) confirmed successful modification of the surface of MCM-41 and quaternization of the nitrogen atom. The activity was verified on a model reaction of styrene oxide with carbon dioxide. The desired styrene carbonate was formed with 100% selectivity in all cases. The influence of pressure of CO_2 and temperature was studied. The pressure of CO_2 didn´t affect the reaction course in range of pressures 0.2 - 2 MPa. However, it was found that high pressures (12 MPa) had an inhibitory effect. Temperature significantly influenced the reaction course compared to the pressure. The yield of styrene carbonate increased with the increasing temperature. Considering efforts to perform CO_2 cycloaddition under mild conditions with the highest possible yield of the desired styrene carbonate, the addition of ascorbic acid to the reaction mixture was studied. Ascorbic acid as a hydrogen bond donor should promote the reaction under ambient conditions, due to the coordination of styrene oxide to ascorbic acid via a hydrogen bond between enediolic hydroxyl protons and the oxygen atom of the epoxide ring, which results in its activation[1].

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GAS-PHASE OXIDATION OF PROPYLENE WITH NITROUS OXIDE OVER SUPPORTED HETEROGENEOUS CATALYSTS

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This contribution concerns the catalytic oxidation of propylene using heterogeneous catalysts. Propylene oxygenates represent industrially important intermediates for manufacture of polyurethanes, polyglycols, acrylates, etc. Direct oxidation of propylene has been studied in recent years as an alternative route to industrial processes: molecular oxygen, nitrous oxide as well as H_2-O_2 have been tested. Gold nanoparticles on TiO_2 are known to catalyze propylene epoxidation with very high PO selectivity (>95%). The epoxidation of propylene with N_2O had been reported with 60%. Recently, potassium halogenide promoted catalysts have shown 13.3% PO yield at 60% selectivity[1,2].

In the present work the catalysts were prepared by deposition of the metal precursor on a support. The effect of the promoter, of aging, of different iron and molybdenum precursors, the synergism between molybdenum and iron, the influence of various oxidizing agents were tested. The catalytic tests were carried out in a fixed bed plug-flow stainless steel reactor.The gaseous products were analyzed online by GS with FID and TCD detectors. The catalysts were further characterized by physico-chemical methods as voltammetry, XRD and TEM. In this work the catalyst preparation, testing of the catalytic activity and the correlation between physico-chemical properties and activities of different catalysts are discussed.

Acknowledgement
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CARBONATES AS A REPLACEMENT OF ACETONE AND CYCLOHEXANONE IN EXPLOSIVE INDUSTRY

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Abstract

Acetone and cyclohexanone are most popular solvents in explosive industry for crystallization of high explosives (RDX, PETN). Cyclohexanone forms relatively spherical crystals suitable for melt-castable formualtions and plastic explosives, acetone is cheap solvent for PETN manufacturing.

Due to toxicity for nervous system and blood alternative solvents can be found in the group of organic carbonates. Dimethyl carbonate is a green solvent with high solvent capacity for RDX and PETN, propylene carbonate is „very green“ non volatile solvent, suitable for RDX crystallization.

Keywords: RDX; PETN; plastic explosive; acetone, dimethyl carbonate, propylene carbonate

EVALUATION OF WASTE PLASTIC PYROLYSIS OIL AS AN ALTERNATIVE FEEDSTOCK FOR STEAM-CRACKING

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Waste plastic pyrolysis is a promising alternative way of chemical recycling of polymer waste. The products include three distinct material streams – non-condensable gas, pyrolysis oil (condensates) and char. The study targets pyrolysis the oil stream, which has no material use in the scheme of a refinery-petrochemical complex. The objective is to evaluate waste plastic pyrolysis oil as a potential alternative feedstock for steam-cracking. It is possible for pyrolysis oil to make up 90 wt. % of the outlet material of waste plastic pyrolysis, therefore it is necessary to find further utilization for this material stream. On top of that pyrolysis oil is a material with properties varying broadly, since its composition is heavily influenced by the type of plastic that is being processed, the technological and operational parameters of the pyrolysis reactor. The demand is therefore to evaluate a large number of different samples to determine whether any of the pyrolysis oils are suitable for the steam-cracking process.

Experimental results suggest a number of pyrolysis oils are promising as a feedstock for the steam-cracking process. Some of them are a great source of olefins such as ethylene or propylene exceeding the production of those olefins as much as 10 wt. % in comparison to traditional feedstock, naphtha. Others are a great source of aromatic hydrocarbons such as benzene or toluene. In that regard different pyrolysis oils can be mixed with traditional feedstock to increase the amount of required products of the steam-cracking process accordingly to the market demand.

The conclusion of the study is that selected waste plastic pyrolysis oils can be used as steam-cracking feedstock and increase its product value. That suggests that pyrolysis and steam-cracking are a promising solution for the environmental problem of waste plastic.

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GAS, COAL, FUEL

OPERATION ANALYSIS OF A TRIGENERATION UNIT

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Economic situation and legal regulations on reducing emissions and cutting expenses trigger the search for new ways to produce energy more efficiently with optimised costs. One of the possibilities in industrial facilities is a trigeneration system combining power generation with heating and cooling. Undoubtedly, there is still an untapped potential in trigeneration unit operation because it is to be optimised case-to-case. Facilities differ in the way heat and cold consumption vary, therefore, a thorough study on the specific facility should be conducted prior to implementing the trigeneration system, followed by monitoring and targeting to ensure its most effective operation. The aim of this study is the examination of current situation in a company operating internal combustion engine-based cogeneration units fired by natural gas in combination with an absorption chiller. In this case, heat energy is consumed both by central heating system during winter and by technology throughout the year, while cooling is used in technology only. A mathematic model is assembled and compared to measured data while addressing the discrepancies in results. Operation problems are targeted and solutions for more efficient unit operation are proposed relying on the developed process hierarchy diagram in form of a decision tree.

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PUSHING THE BOUNDARIES OF SIMULATION-BASED OPTIMIZATION WITH PARALLEL GENETIC ALGORITHM INTERFACE

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Simulation-based single- and multi-objective optimization of industrial processes has been an intensively discussed topic in the last two decades. Modern simulation software such as Aspen Plus usually serves as the simulation environment while modern stochastic methods, such as genetic algorithms, are typical optimization methods of choice. However, simulation-based optimization suffers from extensive computation time due to the need for numerous repetitive simulation runs. In our previous work, an effort to tackle this issue was made by proposing the Parallel Genetic Algorithm Interface (PAGAN) which enables periodic running of parallel simulations, and which was proven to decrease the computation time by 750%. In this work, the potential of PAGAN is vastly expanded by introducing a system of independent parallel simulations. Dubbed PAGAN-II, this interface was used to optimize a 5 MTPA C3MR LNG process with 14 different feedstocks (single-objective optimization, 19 process parameters, 100 individuals, 100 generations). Subsequently, the PAGAN-II performance was thoroughly studied. Results of the analysis have shown that optimization of 14 process alternatives with the respective number of individuals and generations would require approx. 536 hours of computation time (i.e., approx. 22 days) using the standard approach. However, the PAGAN-II algorithm managed to lower the time to 39 hours which translates into a 1490% decrease in calculation time. Furthermore, the study has shown that the increase in relative calculation rate is directly proportional to the number of generations: a standard optimization of 14 process alternatives using a combination of 200 individuals over 200 generations (commonly used in studies) was estimated to last over 143 days, whereas the estimated time using PAGAN-II was 7 days (i.e., a factor of 24).

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POLYMERS, COMPOSITES

VLIV OXIDU A STEARÁTU ZINEČNATÉHO NA VULKANIZACI

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Gumárenský průmysl by se dříve ani dnes neobešel bez reakce natolik zásadní, jakou je vulkanizace. Nejběžnější, sirná vulkanizace, využívá aktivátorů na bázi zinku, zejména oxidu zinečnatého a méně pak stearátu zinečnatého. Jako koaktivátorů se v případě oxidu zinečnatého využívá mastných kyselin, zvláště kyseliny stearové. Ačkoliv se oxid zinečnatý po reakci s kyselinou stearovou pravděpodobně přeměňuje na stearát zinečnatý, tak je chování obou zmiňovaných aktivátorů odlišné. Výzkum se zaměřil zejména na vulkanizační chování směsí aktivovaných oxidem zinečnatým a stearátem zinečnatým. Studován byl průběh vulkanizace, síťová hustota či obsah gelu v síti. Dále byly hodnoceny mechanické vlastnosti, zejména pak tahové.

PRODUCTION AND APPLICATION OF GROUND TYRE RUBBER: A WAY TO INCREASE THE CIRCULARITY OF RUBBER MATERIALS

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The increasing amount of rubber waste, the most of it being constituted by scrapped tyres, is a global issue of today. Therefore, the portion of recycled rubber needs to be increased. Several recycling methods are used commonly, e.g. reclaiming, pyrolysis and material recycling. The latter consists in milling of waste tyres to produce ground tyre rubber (GTR), without being devulcanized. Various milling methods have been applied, producing GTR particles of different sizes and shapes. Some amount of GTR finds application out of rubber industry, e.g. as infill of artificial turf, in construction of roads, playgrounds and buildings, etc. However, the amount of rubber waste utilized in these applications is limited. Therefore, to increase the circularity of rubber material, it is desirable to apply GTR in the production of new tyres. This is not easy, as the compatibility of GTR and rubber matrix is poor, leading to insufficient mechanical properties of the new material. This drawback can be improved by activation of the GTR prior to mixing and by alteration of mixing procedure. The paper brings an overview of GTR production and application.

ENHANCING PROPERTIES OF THERMOPLASTIC MATERIAL: INVESTIGATING NATURAL RUBBER/THERMOPLASTIC STARCH COMPOSITES USING MULTIPLE TECHNIQUES

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The potential of natural rubber (NR) and epoxidized natural rubber (ENR) as modifiers for thermoplastic starch (TPS) as bioplastic is explored in this research. The properties of rubber/TPS composites are investigated using seven techniques: 1) Tensile test, 2) Shore hardness, 3) DMA (T_g) 4) composting 5) SEM 6) water absorption 7) vulcanization, reveal that ENR exhibits better compatibility with TPS, resulting in improved mechanical properties and acts as a compatibilizer for NR and TPS. The study also shows that percolation thresholds may exist in rubber/starch blends, leading to significant changes in performance. The vulcanized ENR/TPS composite exhibits increased tensile strength (from 1.6 MPa to 11.2 MPa) and composting weight loss (56% after 5 weeks), making it a promising sustainable material for packaging and agricultural film applications. The composite materials can be processed by moulding and extrusion. This study has significant implications for the development of eco-friendly materials and offers insight into the potential of NR and ENR as modifiers for TPS in bioplastics.

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POLYOLEFIN STRUCTURE MODIFICATION: FROM BASIC MATERIALS TO POLYMER SPECIALITIES

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Mechanical properties of polyolefins together with their excellent price-performance ratio established them the most used basic plastic materials. Nevertheless, polyolefin´s application field can be still extended by modification of their structure. Polarity increasing of otherwise non-polar polyolefin chains can improve their dyability and compatibility with other materials. Suppression of polyolefin´s crystallinity can make them elastomers. These modifications can move polyolefins from commodity plastics to the field of polymer specialities and increase their value.

In this work, we present several methods for polyolefin structure modification using coordination polymerizations. Nickel and palladium α-diimine complexes provide living coordination polymerization of α-olefins at mild conditions and due to chain-walking isomerization further allow control over the branching of final polymer leading to special polyolefins with supressed crystallization.[1] End-chain functionalization is enabled owing to living character of polymerization (a) by transfer of chain from living growth centre to an organometallic transfer agent followed by cleavage of carbon-metal bond or (b) by addition of polar vinyl comonomer into polymerization system after polymerization of olefin.[2] Late transition metals α-diimine complexes also evince lower oxophilicity and thus enable to prepare in-chain functionalized polyolefins by olefin copolymerization with polar comonomers.[3] Hyperbranched polyolefins with suppressed crystallization can be vulcanized to prepare polyolefin rubber. End-chain functionalized polyolefins can be used for block copolymer synthesis whereas in-chain functionalized polyolefins can be used for graft copolymer synthesis.[4]

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PROCESSING OF PTFE-PEEK POLYMER BLEND IN AIR ATMOSPHERE AND ITS FINAL PROPERTIES

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Poly(tetrafluoroethylene) (PTFE) holds a unique position in the industry as a base material for tribological components, for example, journal bearings or piston rings. The abrasion resistance of pure PTFE is significantly low. For this reason, it is commonly enhanced by fillers (typically glass fibers, bronze, MoS_2, or graphite). It can cause problems since the potential release of fillers is not allowed in specific applications or can cause abrasion of the counterpart. In recent decades, several scientific papers have dealt with a polymer blend based on PTFE and poly(etheretherketone) (PEEK), which may exhibit better wear resistance than individual pure components while maintaining other important properties. The literature mentions mainly tribological properties but no or minimum information about the sintering in an air atmosphere, which is crucial for the industry, where PTFE-based materials are typically manufactured by pressing and sintering. In addition, a typical PTFE sintering process in the air atmosphere causes significant degradation of PEEK.

This work extends the results obtained in the previous work, in which important findings on how the setting of the sintering program affects the degree of degradation of PEEK in the mixture with PTFE were found. The differential scanning calorimetry measurement program for determining the degree of degradation was newly optimized. By this method, the results from previous work were verified. A sintering program that caused almost no degradation of PEEK in the air atmosphere was used for test samples preparation. The tribological and basic mechanical properties were measured and compared to the pure PTFE.

CHIRAL COMPOSITE MEMBRANE FOR ENANTIOMER SEPARATION

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The presence of the modified cyclodextrin in Nafion117® membrane enabled the selective separation of L/D-Tryptophan enantiomers from water. The separation performance is linked to the process used for membrane application. Different experimental set-ups – pertraction, two kind of sorption, and pressure driven membrane separation – revealed the highest performance of membranes in pertraction. Enantiomeric excess reached 18, 22 and 27% in 80 days of pertraction for CD-MIM2, CD-DEG-MIM2 and CD-TEEG-MIM2 membrane respectively. The enan- tiomeric excess as high as 44% was reached in sorption process, using cyclodextrin molecule with a medium chain. However, the experiment took 280 days, and ee close to only 13% corresponds to 80 days of testing time. Corresponding performance of CD-DEG-MIM2 membrane was higher, ee equal 22% and confirm, that pertraction process is more suitable for selective elimination of D-enantiomer Trp from water. While the short spacer in CD modifier is optimal for the preferential sorption, the long spacer was the best for performance for the pertraction and the under-pressure permeation processes.

The pressure-driven permeation process has allowed the operation to be continuous and faster, which has the potential for continuous large- scale production of enantiopure compounds and could pave the way for many more commercial applications, satisfying the considerable demand for large-scale chiral separation techniques. However, low enantiomeric excess was observed in 80 days – 3, 4 and 7%. Reducing the fux of enantiomers through the modified membrane might give more time to the enantiomers to differentiate, decrease the coupling effect and thus increases the enantiomeric excess. After this study we noticed perspectives for future research. The performed separation processes needed long time to achieve required separation factor. When the process is enhanced with pressure to gain in treatment time, we lose in selectivity [1].

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CO_2 SEPARATION USING POLYIMIDE-BASED MEMBRANES

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Membrane technologies for gas separation provide an alternative to conventional separation methods. CO_2 separation from gas mixtures is applied in processes such as biogas purification and raw natural gas treatment. The integration of fillers into the polymer matrix improves the gas separation performance of polymer materials and increases overall process efficiency.

In this work, we focus on the preparation and characterization of mixed matrix membranes (MMMs) based on the new polymer 6FDA-BisP and fillers such as UiO-66, ZIF-8, and MXen. Polyimides synthesized with 4,4-(Hexafluoroisopropylidene)diphtalanhydride (6FDA) have attracted the attention of many researchers due to their excellent permselecitivity promoted by the presence of – CF_3 groups and aromatic rings. Furthermore, due to their structure, the UiO-66, ZIF-8, and MXen particles are suitable for CO_2/CH_4 separation. The 3D configuration forms a high internal free volume that improves the membrane permeability.

XRD, BET, FTIR, TGA, DSC, SEM, and EDS were used to characterize nanoparticles and MMMs. The effects of the mass content and type of inorganic fillers on the separation characteristics and morphology of the prepared membranes have been studied. The permeation measurements of membranes separation efficiency were carried out under different pressures (2, 4, 6, and 8) with a model gas mixture containing CO_2/CH_4 at different ratios (1/1; 3/1; 1/3). The permeability and selectivity of the prepared membranes were calculated from obtained experimental data.

In addition, the Aspen Plus simulation program is used to design the membrane separation process and optimize their working conditions. A simplified model of the membrane separator is demonstrated in the design of a biogas upgrade unit based on two-stage membrane separation. The effect of membrane selectivity and stage cut on energy consumption, methane losses, and purity of methane are presented.

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VOLATILE ORGANIC COMPOUNDS RELEASED FROM PVC WIRE COATING

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Poly(vinyl chloride) is widely used in electrotechnology as insulating material. Its properties are significantly dependent on plasticisers content. In this work we present method for identification of plasticisers in commercially available insulated electrical wire. We quantify and qualify released hydrogen chloride and volatile organic compounds at enhanced temperatures by thermogravimetric analysis, potentiometric titration, and gas chromatography-mass spectrometry system. Changes of glass transition temperatures and mechanical properties caused by enhanced temperatures were measured by thermomechanical analysis. Data shows significant release of hydrogen chloride above 180°C, which has significant effect on insulation and mechanical properties.

SURFACE AND BIOLOGICAL PROPERTIES OF POLYETHERETHERKETONE WITH SILVER-DOPED DOMAINS AS ADVANCED BIOMATERIAL

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The implementation of nanoparticles using an excimer laser opens up new possibilities for creating complex composites. This method offers many opportunities to improve the properties of polymeric materials with metal NPs, especially silver NPs, such as the antibacterial effect on well-known pathogens without side effects on health cells. Our study focused on the anchoring of Ag nanoparticles using a KrF excimer laser (λ=248 nm) in the surface of polyetheretherketone (PEEK). The grid placed just in front of the incident laser beam was used to create the hexagonal structure. Surfaces with Ag-doped domains were characterised by AFM, SEM, and XPS analysis. For subsequent biological tests, the influence of the concentration of released Ag^+ ions was studied by ICP-MS. The antibacterial tests proved the antibacterial activity of Ag-doped PEEK against *Escherichia coli*. Since the final composite is aimed at tissue engineering, the study also included the cytotoxicity tests. In general, our study provides a new and promising strategy for the development of advanced polymeric materials with improved properties for various bioapplications.

PLGA NANOPARTICLES FOR THE LOCAL TREATMENT OF JOINT REPLACEMENT INFECTIONS

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Musculoskeletal infections which commonly accompany orthopaedic surgery are effectively treated with a combination of systemically and locally applied antibiotics in the form of targeted delivery systems with prolonged drug release. Antibiotics administered locally provide a high drug concentration at the target site. This approach benefits from minimizing systemic drug exposure and potentially reduces resistance development[1,2].

The aim of this work was to formulate and characterize vancomycin loaded PLGA nanoparticles (NPs) for the impregnation of bone grafts used as spacers in joint replacements. For formulation of NPs commercial linear PLGA (Purasorb 5002A) and branched non-commercial, experimentally synthesized linear PLGA were used[3]. NPs were prepared by water-in-oil-in-water double emulsion solvent evaporation technique. Polyvinyl alcohol or poloxamer were used for emulsion stabilization.

NP's size, polydispersity and zetapotential were determined using a Zetasizer Nano ZS. Encapsulation efficiency was estimated by UV-spectrophotometry directly by measuring the amount of encapsulated drug after dissolution of NPs in organic solvent and extraction of drug by water. Thermal behavior of blank PLGA nanoparticles and drug-loaded nanoparticles was studied using a DSC. The drug release into the PBS pH 7.4 at 37°C was measured.

As a result of our work, NPs up to 300 nm in size and polydispersity below 0.2 were successfully obtained. The created NPs will be used in further tests after optimalization of other parameters, such as encapsulation efficiency and drug loading.

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BIOPOLYMER FILAMENTS DESIGNED FOR FDM 3D PRINTING OF PERSONALISED ORALLY ADMINISTERED DOSAGE FORMS

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Fused Deposition Modeling (FDM) 3D printing has opened up several new possibilities in various industries, including medicine and pharmaceuticals. The FDM 3D printer, which is versatile, space-saving and cost-effective, can create three-dimensional objects of different geometries, including hollow objects and objects with complex internal structures, according to a computer-aided design (CAD) model.

The main advantage of FDM 3D printing is its flexibility. The CAD model can be edited immediately as needed and cheap prototypes and low-volume products from various materials can be created in a relatively short time. For these reasons, FDM 3D printing is considered in the field of personalised medicine, where it could help with the adaptation of pharmacotherapy according to the specific needs of an individual.

The input material for most FDM 3D printers is a flexible filament of defined thickness made by hot-melt (HME) extrusion. These filaments are remelted during printing to create a unique object, which can also be some type of solid dosage form. Different materials are used for printing, but only a fraction of those can be used in pharmacy to prepare solid dosage forms for oral administration. Our research group is among those who are dealing with this problem. We develop 3D printing filaments based on biopolymers and apply them in printing hard capsules designed for personalised treatment. In the presented work, we mainly focus on HPMC-based filaments containing various biopolymers. These filaments were used for preparing hard capsules tested for their pH-dependent dissolution properties, which are especially important for predicting the behaviour of the dosage form in the digestive tract environment.

COATING MATERIALS BASED ON ACRYLATE LATEXES WITH DISPERSED LA_2O_3 NANOPARTICLES AND TIO_2 PIGMENT, THEIR PREPARATION AND EVALUATION

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The aim of this work was the development of environmentally friendly antimicrobial coatings based on a newly synthesized acrylate water-based polymer dispersion with presented La_2O_3 nanoparticles at a concentration of 1.5% (with respect to the polymer) and TiO_2 pigment prepared by semi-continuous emulsion polymerization. The synthesized coating materials were based on acrylate latexes using a self-crosslinking system of diacetonacrylamide (DAAM) and N-methylolacrylamide (NMA). The influence of nanoparticles and pigments of different chemical composition and particle shape were assessed for the prepared coatings, as mechanical properties, physical properties and antimicrobial properties.
The overall results of the coatings showed acceptable physical properties and mechanical resistance, and thus they could be used as multifunctional coatings. Microbiological tests demonstrated the benefit of cross-linking and the influence of additives on the overall antimicrobial efficiency. The latex cross-linked with NMA achieved the highest antimicrobial efficiency among all latexes, regardless of added additives. For this reason, crosslinking and pigment had the greatest influence on antimicrobial efficacy.

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MODIFICATION OF A NEW PRINTABLE MATERIAL FOR TRIBOLOGICAL APPLICATIONS

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Nowadays, 3D printing technology is so advanced that it finds application in almost every branch of human activity. One of the basic technologies of 3D printing is FDM (fused deposition modeling)/FFF (fused filament fabrication). This method is used for prototyping or small series production of plastic parts. In this industry, the additive FDM technology has enormous potential, because the time to make a prototype is reduced from a few weeks to a few hours, there is a minimum of waste, and in addition, the price of the resulting prototype is only several units to tens of EUR.

One of the factors limiting the widespread use of this technology in the area of design of tribological structural parts is the insufficient supply of materials with satisfactory tribological properties and the frequent necessity of using special printers with a purchase price of several tens of thousands EUR. In this work, a new composite material was developed, which can be processed on almost all common 3D FDM/FFF printers with a purchase price of several hundred EUR.

The composite material was produced by modifying a material based on POM (poly(oxymethylene)) with PTFE (poly(tetrafluoroethylene)). This material is the result of previous research activity. Two fillers were used for the modification – carbon and basalt fibers. Two mixtures were prepared by compounding the fillers with the base material. Filaments were prepared from the mixtures, which were checked for homogeneity. This was followed by determination of parameters for 3D printing, adjustment of the printing pad and verification of printability. The final step was the printing of test specimens to verify the mechanical and tribological properties.

EFFECT OF CATALYTIC SYSTEM ON STRUCTURE OF ETHYLENE/PROPYLENE COPOLYMERS

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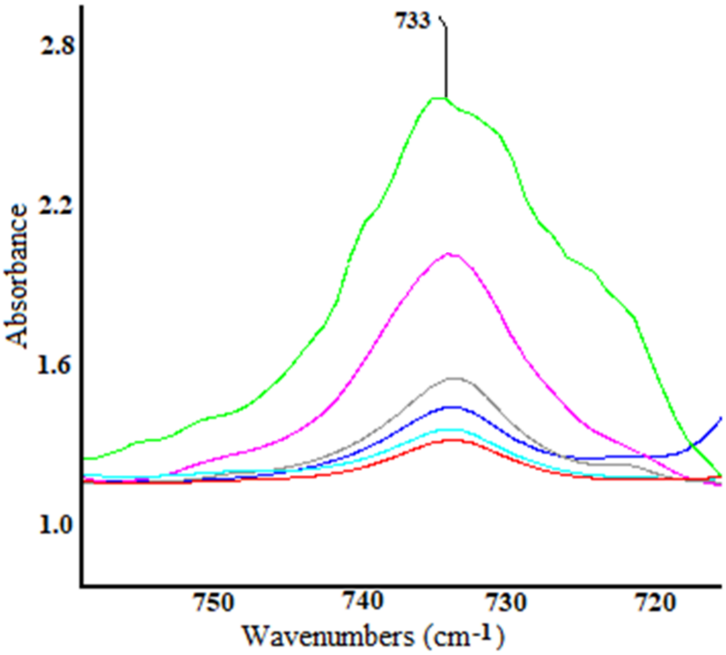
The research is focused on the structural study of ethylene-propylene copolymers (E/P copolymers) produced by gas phase polymerization in stainless-steel batch reactor. The aim of the work was to determine the effect of different catalysts on the distribution of ethylene units in the resulting material. Three E/P copolymers with the same content of ethylene were prepared on commercial Ziegler-Natta (ZN) catalysts, which differed in the structure of the internal donor (ID). One ZN catalyst contained diether ID and second phthalate ID.

The E/P copolymers were fractionated using Temperature Rising Elution Fractionation (TREF) method, which separated the original samples into fractions according to their crystallization ability.

TREF analysis revealed that the incorporation of ethylene into growing polypropylene chain is dependent on the catalytic system. Using structural analysis methods, the difference between copolymers structure was described and it was found that the catalyst with the phthalate internal donor supports the creation of ethylene blocks capable of crystallizing, while the catalyst with diether ID doesn't have this ability. As it is know from literature, in the case of phthalate-based catalysts, the effect of alkoxysilane external donor (ED) on the incorporation of ethylene units into growing polypropylene chain must be included because ED replaces the phthalate internal donor, which is extracted from the catalyst by reaction with triethylaluminium (TEA) co-catalyst. In the case of diether-based catalysts, the external donor doesn't play such an important role, because its extraction from the catalyst by the reaction with TEA is limited. We assume that the alkoxysilane compound in the case of the phthalate-based catalyst and the diether compound in the case of diether-based catalyst are the main reason of the different incorporation of ethylene units into growing polypropylene chain.

Figure 1: FTIR spectrum of sample R1877 and its fractions after TREF fractionation (●F30; ●F90; ●F100; ●original; ●F110; ●F160). The ethylene content of the individual fractions was confirmed by a rising peak at 733 cm^{-1}.



MODELING OF GAS-PHASE POLYMERIZATION PROCESS OF PROPYLENE - REACTION KINETICS

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The gas-phase kinetic polymerization model of propylene was constructed for the modelling of polypropylene production in the industrial polymerization reactor in ORLEN Unipetrol, Litvínov. It was based on the deconvolution of GPC curves, considering and using a 4-active site catalytic model, which describes the overall production of polypropylene well both in semi-batch and in industrial polymerization reactors.

The model is comprised of two principal dependences of catalyst activity on:

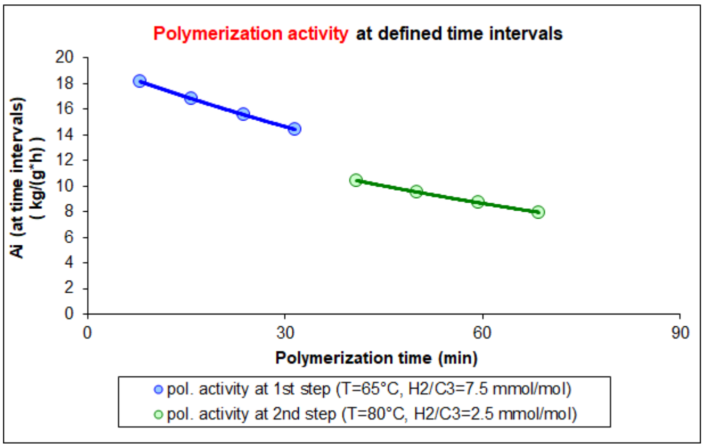
- polymerization temperature (4 temperatures in the range: T = 65 - 95 °C) and
- hydrogen concentration (8 hydrogen concentrations in the range: H2/propylene = 0.120 - 120 mmol/mol).

The complete model thus comprised of 4 x 8 combinations of these polymerization parameters and 32 final polypropylene materials intended for GPC deconvolution and the calculation of kinetic parameters.

The kinetic polymerization model can be used in the following ways:

- For the on-line prediction of polymerization yield and activity.
- For the optimization of reactor productivity.
- Later as a part of a more complex model for the calculation of the melt index (Mw) and MWD distribution of produced homopolymer PP materials.

Figure 1: Simulation of influence of polymerization temperature and hydrogen concentration in propylene (H2/C3) on catalyst activity in 2-step homopolymerization.



ISOLATION AND ANALYSIS OF GRAPE SEEDS LIGNIN FOR POTENTIONAL APPLICATION IN POLYMERIC BLENDS

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The utilization of waste materials is a crucial aspect of the circular economy. In this regard, this work focuses on processing agricultural waste, particularly from wineries, to isolate lignin. Lignin is a widely occurring biopolymer found in the cell walls of vascular plants. Nowadays, lignin is primarily obtained as a by-product of the pulp and paper industry and is directly utilized for energetic purposes. However, lignin has much broader application potential thanks to its unique properties such as antioxidant activity, antimicrobial properties and UV protection. This work deals with the isolation and analyses of lignin obtained from grape seeds. The isolation was carried out using the soda pulping method with sodium hydroxide. This method is advantageous because it yields sulfur-free lignin. The solubility of the isolated lignin fractions was assessed using various organic solvents, with the choice of solvent being crucial for further application. A comparison of these solvents revealed that dimethyl sulfoxide had the highest solubility of isolated lignin at 95%. Solubility was then confirmed by particle size analysis. The antioxidant activity of lignin was assessed by the ABTS radical scavenging method, as it can be beneficial for lignin applications. The antioxidant properties of lignin are related to its total phenolic content, which was determined spectrophotometrically.

Lignin has numerous potential applications, including manufacturing green chemicals, adhesives, and fillers for polymers. This study also aimed to prepare blends of polyhydroxyalkanoate with grape seeds lignin. Adding 1 wt% grape seeds lignin enhanced Young's modulus and tensile strength of the blends by 60 MPa and 21 MPa, respectively, while maintaining the elasticity of the material. Furthermore, the lignin improved the degradation onset temperature by 15°C, which could help overcome challenges in processing polyhydroxyalkanoates.

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SOLVENT BASED RECYCLING OF PLASTIC WASTE: ADDITIVES REMOVAL

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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 synthetic 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. However, they are full of polymer additives containing a scale of problematic elements for recycling (nitrogen, sulfur, chlorine or fluorine). Decolorizing can enrich the value of plastic waste and the removal of all polymer additives is the aim of this contribution, where we focus on PE and PP to develop the purification and refining process methodology.

Our first experiments were conducted to probe the possibilities of creating polymer solutions and handling them with extraction apparatus. Assembled stirred pilot apparatus is designed to set various experimental conditions (pressure up to 30 bar and temperature up to 150 °C). The apparatus is equipped with three glass windows for visual control, instrumental check of polymer–solvent mixtures, and determining their cloud point.

Pilot experiments were conducted with commercial plastic waste following the literature [1]. The experiments were successfully repeated, but plastic waste is not suitable for systematic analysis due unknown composition of used polymer additives. Therefore we created plastic waste samples with a known amount of specific additive to calibrate the instrumental FTIR and Raman spectroscopy method.

The initial results were simply compared as decolorized/not decolorized, but now we are using spectroscopy methods to determine proper conditions and solvent-antisolvent-polymer system. We starting with screening of a large number of solvents, but we aim to use only non-toxic nature-friendly chemicals with their subsequent regeneration.

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MESOPOROUS ADSORBENTS FOR CO_2 CAPTURE BASED ON AMINE-FUNCTIONALIZED SILICA AND ORGANOSILICAS

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Carbon dioxide (CO_2) capture and storage have been suggested as an effective strategy to reduce global greenhouse gas emissions. In recent years, many studies were carried out to develop highly efficient materials, such as zeolites, porous carbons, metal-organic frameworks (MOFs) and metal oxides for capturing CO_2. In addition, interest in studying amine species grafting with mesoporous materials to improve CO_2 capture by amino groups have increased tremendously. These modified materials provide excellent CO_2 uptake capacity, fast adsorption kinetics and easy regeneration with stable cycling performance. Mesoporous silica is a very popular solid adsorbent for gas- and liquid-phase applications including CO_2 sorption. Recently, porous solid adsorbents such as silica have been modified by the amine-containing compounds to increase their affinity toward CO_2.
Herein, CO_2 adsorption was investigated on amine-functionalized mesoporous silica and periodic mesoporous organosilica samples. Hexagonally ordered mesoporous SBA-15 and benzene-PMO (BPMO) samples were prepared and functionalized by amine-containing modifier TSPED (N-[3-(trimethoxysilyl)propyl]-ethylenediamine). Nitrogen adsorption isotherms showed that these samples featured mesostructured, high surface area, and narrow pore size distributions. N-[3-(trimethoxysilyl)propyl]-ethylenediamine-modified silica samples exhibited substantially higher CO_2 uptake compared to original material; maximal values for SBA-15_A ~3.1 mmol/g, for BPMO_A ~2.5 mmol/g and SBA-15-BTEP_A ~2.5 mmol/g, measured on a volumetric adsorption analyzer at 25 °C. The amine-modification also significantly improved the CO_2/N_2 separation properties of all prepared silica samples (e.g. SBA-15 from 14 to 86 for pressure 1 bar).

Acknowledgement

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CO_2/CH_4 SEPARATION BY HYPERBRANCHED AND DENDRON-CONTAINING POLYMERIC MEMBRANES

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Due to environmental, operational and economic impacts of acid gases such as CO_2, H_2S, NO_x and SO_x, development of new separation technologies with enhanced efficiency and low capital cost is an emerging demand in the near future. Membrane separation process is considered a promising technology for gas removal and recovery owing to its reasonable cost, good selectivity and lower environmental impact. The development of innovative membranes having both high gas permeance and selectivity becomes very important.
Herein, the idea of dendron-containing polymers (dcPs) to preparation of effective membranes for CO_2/CH_4 separation is presented. Incorporation of groups such as amine or phosphonium into the polymer structure can be expected to increase the affinity of the material to CO_2, and thus to improve the CO_2/CH_4 selectivity of prepared membranes.

Acknowledgement

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SORTING OF PLASTIC WASTE UTILIZING TRIBOELECTRIFICATION AND SUBSEQUENT ELECTRIC FIELD SEPARATION

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The separation of plastic materials is crucial for their material or energy-content recycling, i.e., for making a positive economic value from useless waste. None of the separation methods for plastics can be used universally. We are focusing on the efficiency improvement of triboelectric separation of plastics: this method is low cost, can be automated, utilizes no chemicals, and can separate even black-pigmented plastics.

The triboelectric separation consists of three main steps. In the first step, plastic waste is grinded into small pieces. Then, the charge is generated on their surface by tribocharging. Lastly, charged pieces are separated during free fall between electrodes in the electrostatic separator. Triboelectric separation is based on the phenomenon that each plastic material obtains a different electrostatic charge by friction contact with a proper counter-material. Selecting a counter-material is the most challenging task in designing a triboelectric separator, as it plays a crucial role in controlling the charge obtained by individual plastic pieces, thus, affecting the purity and yield of this method.

Here, we present the study of essential parameters: chemical composition, grinded waste size, and triboelectrification type. We are also studying the effect of the external electric field present in the charging cell or utilization of corona discharge; these process modifications address several key issues in the scale-up of this method: long charging times and possible depletion of charge carriers during continuous operation.

Lastly, we present a case study of sorting unwanted halogenated waste (PVC) from a 3-component mixture (PVC-PET-PP). In three simple separation steps, we managed to sort out the PVC with purity up to 91 % at 88% recovery.

OIL,
PETROCHEMICALS,
BIOFUELS

KEY TRENDS AND STRATEGIES IN THE OIL AND PETROCHEMICAL INDUSTRY

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The number of refineries in Europe is steadily declining (89 refineries, capacity 663 $Mt \cdot y^{-1}$ of crude oil by 2022) and refinery equipment is aging in contrast to the Middle East and Asia, where large investments are being made. Efforts to save energy for economic reasons are now being transformed into operational and product decarbonization, to counteract negative climate change as a fundamental imperative. Some refineries are being transformed into biorefineries as a transition towards the circular economy (Marathon Petroleum Martinez refinery is the last one). There is a drive to shift the feedstocks pool and utilities towards components produced from agricultural residues, municipal wastes, and recycled plastics and scrap tires. Refinery of the future (Honeywell), zero-emission technologies (KBC and Lummus), and energies and products with low carbon content are concepts discussed now. New environmentally friendly technologies (Honeywell, nViro; KBC Hydro-PRT), innovative technological schemes (Honeywell, Integrated Olefins Suite), new equipment (Watlow, electric heating), and state-of-the-art catalysts (golf balls, ionic liquids) are being developed. The drop-in concept will be important in the transition phase to decarbonized products. E-fuels / E-chemicals represent a way of joining various sources of carbon dioxide and green hydrogen for the synthesis of methanol (direct utilization, synthesis of gasoline or alkenes) or Fischer-Tropsch synthesis to synthetic crude oil and represent an example of the increasingly close integration of the refining and petrochemical industries. The role of digitalization increases for planning, optimization of production, predictive maintenance (development of digital twins), logistic, workforce, safety, and protection of the environment. Large software companies (AspenTech, Microsoft) are involved in these trend. Change in staff mindset, strong leadership, proper master planning of future activities and new investments will be important in preparing entrepreneurially successful strategies.

ZERO EMISSION REFINERY: REALITY OR DREAM?

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Oil refining is an energy-intensive industry. Addressing its operation without harmful emissions in 20XX will be a major challenge. There are the following pathways to reduce emissions from refineries: digitalization, upgrading technologies to less energy intensive, increasing the concentration of carbon dioxide in the flue gases by combustion with oxygen, sequestration and chemical utilization of carbon dioxide (CCSU), use of green hydrogen as fuel, and electric heating. These pathways can be used in parallel. Electricity already contributes significantly to the refinery's energy consumption. The use of green electricity for heating will be advantageous due to zero emissions and the ability to substitute different energy sources in the refinery, such as fuel gas of various composition and external steam of various pressure. Appropriate electric heating is already available. Therefore, a case study of electric heating utilization on decarbonization of operation was examined from a typical FCC conversion refinery with a capacity of 6 Mt·y^{-1} was examined. Three cases of carbon dioxide elimination were considered (Table 1).

Table 1: Total energy, electricity and carbon dioxide balance for analysed cases

Case description	Total energy consumption (GWh·y^{-1})	Consumption of electricity (GWh·y^{-1})	Export of energies (GWh·y^{-1})	CO_2 refinery emissions (kt·y^{-1})
Current configuration	540.1	338.8	-800.6	1138.7
Case 1 + Replacement of external steam by electric heating	4540.1	589.3	-800.6	1138.7
Case : Case 1 + Replacement of refinery gas by electric heating (export of refinery gas)	4540.1	2494.0	-2705.4	756.4
Case 3: Case 2 + use of FCC off-gas CO_2 for 562 kt·y^{-1} methanol production, utilizing green H_2	10393.4	8347.4	-2705.4	0* (10.9)

* Note: approx. 11 kt·y^{-1} carbon dioxide will be emitted for security reason: off-gases incinerator

Case 1 reduced carbon dioxide emissions by external steam supplier (-55.9 kt·y^{-1}). In case 2 refinery gas was supplied to a local electricity and heat producer replacing there import of natural gas, with reduction of carbon dioxide emissions at refinery gate approx. 34 %. Case 3 targeted zero carbon dioxide emissions. Carbon dioxide from the FCC regenerator was used to produce methanol. Due to the need for 'green hydrogen', electricity consumption increases significantly. Zero emission refinery will not be a dream assuming technological use of coke from FCC.

POTENTIAL FOR USE OF SIDE STREAMS IN THE PRODUCTION OF DICYCLOPENTADIENE

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During the test run of the unit for dicyclopentadiene (DCPD) production based on light pyrolysis gasoline (LPyGas) technology, initial experience were obtained. The process data verified the previous research assumptions accompanying the development of the technology and also show the potential for various process optimization. The maximum effectiveness of the DCPD isolation from LPyGas should be achieved by optimizing the operating conditions with the aim of minimizing direct losses of DCPD to backflow gasoline and at the same time by efficient use of side streams with a high content of DCPD. Finding the commercial use of methyldicyclopentadiene (MeDCPD) which is produced as a by-product of DCPD production represents the example of evaluation of one from a group of hydrocarbons originating from the Steam cracker and apparently also the potential for expanding the DCPD unit to include a part of MeDCPD stream processing. The main goal of optimization is primarily to find key operating conditions for precise control of purity and other parameters of the produced DCPD and MeDCPD – especially the color and impurities.

HIGH TEMPERATURE REMOVAL OF HALOGENATED COMPOUNDS FROM PYROLYSIS OF WASTE PLASTIC ON SOLID SORBENTS

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Chemical recycling offers utilization of waste plastics not suitable for mechanical recycling to products with higher added value. Chemical recycling of plastic is alternative for substituting current fossil feedstock in petrochemical industry or refineries.

Plastics can contain some undesired components that can cause problems in subsequent technologies and possible utilization as fuel such as catalyst damage or corrosion. These compounds consist of chlorine and other halogens which can transfer to final product. Therefore, it is necessary to reduce content of these compounds to acceptable level. One of the possible ways to remove halogenated compounds is high temperature adsorption on solid sorbents.

This work focuses on high temperature removal via basic sorbents in model mixture including hydrocarbons, hydrogen chloride and other compounds. Experiments were performed in laboratory scale apparatus. Model mixture allowed us to precisely describe and monitor sorption efficiency and changes in model substances used. Perspective sorbents from previous experiments with dry gas were used for subsequent experiments in wet gas (including water vapour) which can affect sorption properties. Relatively inexpensive sorbents were positively affected by presence of water vapour. Final purpose is to transfer laboratory results in larger scale that is closer to industrial application.

COFFEE WASTE AS A SOURCE OF OIL FOR BIODIESEL PREPARATION BY HETEROGENEOUS TRANSESTERIFICATION OVER La-Ni/MgAl MIXED OXIDES

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Biodiesel is an alternative to commonly used diesel fuel. The preparation of biodiesel produces a significantly lower amount of emissions, its resources are renewable and its properties are almost identical to diesel fuel, which enables mixing of biodiesel with diesel fuel or complete replacement. Biodiesel can be prepared by transesterification of triacylglycerides with methanol over suitable catalysts. Heterogeneous transesterification offers a lot of advantages in comparison with homogeneous. Easier separation of products from heterogeneous catalyst, possibility of catalyst regeneration and lower sensibility to free fatty acids present in vegetable oils or other sources. Free fatty acids are mostly present in waste cooking oils or other oils from waste such as coffee waste. Worldwide, more than 7 milliard tons of coffee waste are produced. From coffee spent grounds is possible to obtained oil, which is suitable for biodiesel preparation but have high amount of free fatty acids and other impurities. Hydrotalcites are great source for mixed oxide preparation. Into its layered structure is possible to incorporate different types of cations and anions. Choice of cations causes changes in physic-chemical properties as well as in catalytic activity in transesterification. Combination of incorporation of divalent and trivalent cations into basic Mg/Al hydrotalcites such as La and Ni caused improvement of catalytic activity of mixed oxides in transesterification. Catalyst activity and resistance to free fatty acids content was tested in transesterification of different types of refined coffee oils with different acid numbers. The content of FAME in biodiesel prepared oved La-Ni/MgAl mixed oxides by two-step transesterification of coffee oil was higher than 99 wt.%. The activity of catalyst in waste oil with high content of free fatty acids was high and the content of FAME meets the European standards.

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EFFECT OF CARBON CHAIN LENGTH AND SHAPE OF HYDROCARBONS MOLECULES ON CATALYTIC CRACKING AND AROMATIZATION OVER HZSM-5 CATALYSTS DURING CATALYTIC PYROLYSIS OF POLYOLEFINS

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The catalytic dehydroaromatization of alkanes to aromatics [1] have attracted considerable attention of chemical industry, because it can be used for the upgrading of low-cost alkanes into high added-value aromatics, such as benzene, toluene, and xylene (BTX). The same process occurs during thermo-catalytic pyrolysis of plastics, especially in polyolefin treatment, where polymer chains are cracked producing aliphatic hydrocarbons which then undergo olefination and dehydroaromatization. The aromatic yield and selectivity in thermo-catalytic treatment of waste polyolefins can be improved by optimizing the catalyst properties as well as the process parameters. For this purpose, it is important to gain an enhanced understanding of the dehydroaromatization of individual hydrocarbons that result from initial cracking of polymer chains.

In our recent work we have reported thermo-catalytic pyrolysis of virgin polyolefins over HZSM-5 zeolite catalysts investigating the influence of catalyst acidity, operation mode and process parameters on the production and selectivity of aromatics [2,3]. The present work is a follow-up study aiming at investigating the influence of different carbon chain length and shape of individual hydrocarbons on the product distribution in catalytic cracking and dehydroaromatization process. It was shown that the size and type of hydrocarbon chains strongly influence the conversion as well as aromatic selectivity. This is directly dependent on the ease of diffusion of the individual molecules through zeolitic pores when reaching the active centers. Moreover, since branched chain hydrocarbon (main cracking products of PP pyrolysis) have restricted diffusion in micro pores of zeolite catalysts, zeolites with hierarchical porosity (e.g. micro-meso and micro-macro) can be interesting catalytic materials for their processing.

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SLUDGE FORMATION DURING LONG-TERM STORAGE OF VARIOUS TYPES OF CRUDE OIL

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European legislation mandates each Member State to manage emergency oil stocks for 90 days of average consumption. The importance of strategic oil stocks is evident in the context of political and economic circumstances, not least in the last few years. Long-term storage brings a need to maintain not only the quantity but also the quality of the oil. The greatest changes in quality are caused by the separation and sedimentation of some oil fractions. Apart from water and solid particles, these are mainly particles containing high-molecular-weight n-alkanes. Preventing or removing and disposing of sludge from storage tanks has financial costs associated with increased energy consumption, loss of stored medium, operation of cleaning technologies, and blocking capacity during tank shutdowns.

This work aimed at experiments simulating oil sedimentation in a laboratory model at a 1:20 scale down compared to a real storage tank. The model storage process was evaluated by determining the content and distribution of n-alkanes in the resulting sediment layers. The paper discusses the quantity and quality of the formed sediments in relation to the storage temperature and selected physicochemical parameters of the oil, including the microscopic evaluation of paraffin particles. The intensity of sedimentation depends not only on the amount of sedimenting material but also on the storage temperature, which undergoes seasonal changes on an operational scale. Therefore, in addition to tests at a constant temperature, tests simulating the annual temperature variation in real storage tanks were also performed. A low tendency to deposit formation at lower temperatures was observed, although at these temperatures a higher amount of solid paraffin is present in the samples. Despite the limitations in predicting the sedimentation, the findings have contributed to explaining the behaviour of long-term stored oils, which is also relevant for the selection of oil types suitable for strategic reserves.

POTENTIAL OF MIXED OXIDES IN VALORIZATION OF ETHANOL TI ADD VALUE CHEMICALS

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Mixed oxides are group of promising materials which are implemented in many applications, such as antacids, adsorbents, catalysts etc. These materials have found a wide spectrum of applications due to their changeable properties, such as the change of a composition, calcination temperature and methods of precursor (LDH) synthesis. Moreover, the low expenses and not complicated synthesis of these materials allow their easy commercialization and application in catalysis.

With development of the society and increase of the energy and materials consummation, a higher production of CO_2 leads to global warming. Therefore looking for the new processes is needed to process the biomass to biofuel and chemicals. One of the promising feedstock prepared from biomass is ethanol. Ethanol could be converted to different compound as ethylene, butene, acetaldehyde, ethyl acetate, butanol, hexanol etc. by variable processes. The higher alcohols, mainly butanol, could be prepared by Guerbet reaction. Guerbet reaction consist of three consequent reactions (dehydrogenation, aldol condensation and hydrogenation), where the different types of active sites are applied. The key role in this process has catalyst with basic species, which enables the dehydrogenation/hydrogenation reaction on metal species and subsequent aldol condensation. The easy variability of mixed oxides predict the final performance for Guerbet reaction.

The mixed oxides with transition metals (Ni, Cu, Co) were tested in fixed bed stainless steel microreactors at three reaction temperatures (280, 300 and 350 °C). The catalysts were characterized for determination of the structural (XRD), textural (N_2-physisorption), acid-based (TPD-NH_3, CO_2) and redox (TPR-H_2) properties. It was found, that the presence of the transition metal improved the conversion of the ethanol. Also, our study proved that the transition metal improved the dehydrogenation performance at lower temperature compared with basic catalysts, where the temperature above 400 °C are necessary. However, the presence of transition metal strongly influenced of the selectivity to higher alcohols, where at the higher temperature than 300 °C, a gasification was observed.

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EXTRACTION OF CYCLOALKANE−AROMATE SYSTEM USING IONIC LIQUID

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In today's industry, aromatics have a widespread use, e.g. in the plastics, food, pharmaceuticals and cosmetics production. Fossil sources serve as a source of aromatics, they should be separated. Due to the similar boiling points of the mixture components, liquid phase extraction, extractive or azeotropic distillation is used for this purpose. For the above processes, selection of a suitable extraction solvent is crucial bearing in mind that some requirements on the extraction solvent contradict each other and a compromise should be found regarding the extraction solvent selectivity and capacity. Nowadays, ionic liquids are considered substitutes for organic solvents in extraction processes. As an extraction solvent for the separation of cycloalkane–aromatics mixture, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMim][NTf_2]) was tested. Methylcyclohexane represents cycloalkane in the model mixture, while toluene and *m*-xylene represent aromatics. A routine simulating extractor operation was developed in the Matlab environment. Variation on the number of theoretical contacts with the relative ionic liquid consumption in the extraction equipment was investigated, assuming that the solvent demand is 1.2 times the minimum one. The optimization criterion was the prescribed maximum aromatics content in the resulting raffinate (0.005 mole%). [EMim][NTf_2] ionic liquid showed potential in the aromatics' separation from the model cycloalkane−aromatics mixtures. The principal advantage of this solvent is that it is practically not present in the raffinate (ionic liquid content below 0.002 mole%). When comparing the separations of toluene and *m*-xylene from their mixtures with methylcyclohexane, comparable yields of the extracted component were obtained, although the relative solvent consumption for the separation of *m*-xylene was 1.4-times higher than the value obtained for toluene separation. On the other hand, the difference in the number of theoretical contacts required for the two hydrocarbon mixtures separation is minimal. For the MCH−toluene and MCH−*m*-xylene mixtures separation, 10 and 9 theoretical contacts are necessary, respectively.

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TERTIARY RECYCLING OF WASTE POLYPROPYLENE IN THE TWO-STAGE REACTOR SYSTEM

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Abstrakt

A bench-scale reactor with continuous feedstock dosing (2L volume) was used for the waste polypropylene cracking tests. The reactor itself is based on a spouted-bed concept, a carrier inert mixing gas (nitrogen or CO2 was used) is injected into the bottom of the reactor and dispersed through a nozzle located at the bottom of the conical part of the reactor. Sorted packing materials were used as waste PP, which was crushed and regranulated.

The shape of the temperature profile in the reactor, the carrier gas flow rate, which influences the residence time of the products in the reaction zone, as well as the partial pressure and the feedstock feed rate, had the greatest influence on the distribution of the waste PP cracking products. The proportion of gas increases with increasing temperature from 420 to 460oC insignificantly from 7 to 14 wt.% depending on the hydraulic conditions in the reactor. Decreasing the carrier gas flow rate increases the gas fraction by 1% point. In terms of composition, the gas contains the highest concentration at propylene 56-63 wt.% and iso-butene 10.20 wt.%. The major product of thermal cracking of PP in a conical reactor is liquid hydrocarbons in the range of C5 to C40. The liquid fraction was yellow in colour and clear in the case of native PP. The higher boiling fractions of the product from the first reactor were cracked in a second reactor with a piston flow in the presence of a catalyst (clinoptilolite and alumina). In the second reactor, cracking of hydrocarbons with boiling points above 360o C continued and the concentration of heteroatoms was reduced.

The PP thermal cracking products contained a mixture of alkanes, alkenes and alkadienes in a 1:17:1 ratio, with low concentrations of cyclanes and aromatics. This observation was matched by the high bromine number and extremely low crystallization temperature values of the PE fraction (less than -81oC).

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BIODIESEL PREPARATION BY HETEROGENOUS TRANSESTERIFICATION OF DIFFERENT TYPES OF NON-FOOD, WASTE AND VEGETABLE OILS OVER MIXED OXIDES

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Hydrotalcite (part of double layered hydroxide – LDH) has a special layered structure, which is composed of octahedral cationic layers and interlayer space with anions and water. By calcination of hydrotalcite crystal structure over 450°C is possible to obtained mixed oxide amorphous structure, which have better catalytic properties and is more active in biodiesel preparation. Biodiesel is commonly prepared by homogeneous transesterification of vegetable oil with methanol. Homogeneous transesterification have drawbacks such as difficult separation of catalyst and biodiesel, which cause large water consumption when washing the catalyst from biodiesel. Based on the used source for biofuel production, biofuels are divided into first, second and third generation. Nowadays mostly first generation of biofuels are produced, when edible vegetable oils are used. Replacement of edible oils by non-edible, non-food or waste oil producing second generation of biofuels. For comparison of activity of mixed oxide in transesterification for biodiesel production, different types of oils were used. From edible oils, corn and sunflower oils were used. As an alternative oil, Camelina sativa non-food oil was tested. Camelina sativa is a plant, which needs fewer fertilizers and minerals to grow and is relatively resistant to drought. From non-edible oils was also used for biodiesel preparation, refined Hemp oil in cosmetic quality. Coffee oil obtained by extraction from coffee waste was used as a representative of waste oils. Different oils have different compositions and content of impurities. The transesterification of oils was performed in batch reactor over mixed oxides containing lanthanum and nickel. As a main qualitative parameter of prepared biodiesel, content of FAME was measured. The impact of oil choice for transesterification was observed. Activity of catalyst was confirmed in transesterification of waste, non-edible, edible and cosmetic oil.

Acknowledgement
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AROMATIZATION OF n-HEXANE OVER HIERARCHICAL Ga- and Zn-ZSM-5 ZEOLITES

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Zeolites are crystalline aluminosilicates of alkaline elements, rare earth elements or other monovalent or multivalent metals, belongs to the microporous materials. These materials display several unique properties, due to which they are applied in catalysis. Despite their numerous advantages, zeolites also display diffusion limitations for branched molecules and transport of reagents with size like the size of the micropores is difficult. This leads to a situation in which only the external part of zeolite grain takes part in catalytic reaction while the interior remains catalytically inactive. Therefore, works have begun on the synthesis of zeolites with hierarchical porous structure which display secondary porosity i.e. show the presence of at least one additional pore system, mainly in the mesopore range. Such solution aims to facilitate access of larger reagent molecules to active sites of the material while simultaneously maintaining acidity and crystallinity of zeolites. Shortening the length of diffusion path due to the reduction of crystal size (obtaining both nanocrystals and nanolayered zeolites) causes increase in catalyst lifespan. Introducing additional porosity (meso-, macro-) also shortens the diffusion path, thus minimizing the possibility of catalyst deactivation. Hierarchical zeolites have already found application in, among other things, catalysis, in such reactions as: alkylation, isomerization, transformation of methanol to hydrocarbons, aromatization, condensation or catalytic cracking. This work focuses on the synthesis and characterization of hierarchical zeolites ZSM-5 and their application in an aromatization of n-hexane. Recrystallization of zeolite ZSM-5 did not have a negative effect on the physicochemical properties of the prepared catalysts. The treatment and the loading of the active metal caused a significant increase in the n-hexane conversion more than 2 times, while the content of aromatic hydrocarbons increased almost 9 times.

SYNTHESIS
AND PRODUCTION
OF DRUGS

KONJUGÁTY PROTILÁTKA-LÉČIVO, SPOJENÍ VELKÝCH A MALÝCH TERAPEUTICKÝCH MOLEKUL V ONKOLOGII. ELEKTRONOVÁ DIFRAKCE

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Konjugáty protilátka-léčivo (Antibody-Drug Conjugates) jsou velmi aktuální terapeutickou skupinou kancerostatik. Tvoří je monoklonální protilátka (mAb), nejčastěji typu IgG, na kterou je přes vhodný linker (kovalentní řetězec) konjugována jedna nebo více molekul cytotoxického léčiva. Konjugovaná forma léčiva má výrazně nižší toxicitu než forma volná, kterou v terapii nelze užívat samostatně. Strukturně a funkčně důležitými parametry ADC konjugátů jsou: sekvence aminokyselin v mAb, posttranslační modifikace mAb, pozice vazby mezi léčivem a mAb a průměrné zatížení mAb léčivem. Tyto parametry se určují mimo jiné strukturními technikami, především MS, RTG difrakcí, kryoelektronovou mikroskopií a elektronovou difrakcí.

Databáze SÚKL registruje zatím 9 ADC konjugátů pro použití v onkologii. Vzhledem k tomu, že možných kombinací párů protilátka-léčivo je obrovské množství, očekává se jejich „boom“ a až čtyřnásobný nárůst prodejů do roku 2025. U ADC konjugátů se používají humanizované nebo plně humánní mAb, především z důvodu nižší imunogenity. V krevní cirkulaci směřuje ADC konjugát specificky k antigenu exprimovanému na povrchu nádorové buňky. Linker (vazebná spojka) mezi protilátkou a léčivem musí být stabilní v prostředí krevní cirkulace a teprve až po internalizaci konjugátu být v cílové nádorové buňce zcela degradován nebo zůstat vázaný na léčivo po degradaci proteinové části konjugátu (tzv. štěpitelné nebo neštěpitelné linkery). Následně léčivo způsobí různými mechanismy apoptózu nádorové buňky. Léčiva použitá v ADC konjugátech 2. generace byla až 1 000x toxičtější než chemoterapeutikum doxorubicin a jednalo se především o deriváty auristatinů a maytansinů. V současné 3. generaci vyvíjených konjugátů se zkouší i méně toxická léčiva na bázi kamptothecinů, amanitinů aj. Léčivo s linkerem je k mAb připojeno pomocí různých biokonjugačních metod. Zde se uplatňuje celá škála technik syntetické chemie, přičemž biokonjugace může být buď nespecifická nebo specifická. Konjugovatelné jsou především periferní aminokyseliny mAb - cystein, lysin, histidin, tyrosin, glutamin a redukované disulfidové můstky mezi dvěma těžkými nebo mezi těžkým a lehkým řetězcem. Pro specifickou konjugaci byly vyvinuty např. techniky glykoinženýrství, založené na N-glykosylaci mAb na asparaginu (N297).

Konjugační techniky, ale i syntéza „nahé“ humánní mAb jsou předmětem utajovaného „know-how“ řady progresivních firem a laboratoří, které v oblasti ADC konjugátů působí, např. Seattle Genetics, Genentech, ImmunoGen, Regeneron, AbzenaBiosystems, aj.

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ROLL COMPACTION PROCESS DEVELOPMENT AND TRANSFER AIDED BY COMPACTION ANALYZER

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Roll compaction (RC) is a technology for dry granulating pharmaceutical powders which was never massively adopted for pharmaceutical tablet production due to worse performance of produced granulate in comparison to granulates produced by high-shear wet or fluidized bed technique. Nowadays it is gradually attracting more attention as it can save manufacturing costs and it can, as an inherently continuous process, nicely fit into the continuous manufacturing production lines. The process development and technology transfer of the roll compaction is relatively difficult due to the complex nature of the underlying phenomena. Our contribution presents a hybrid approach how to deal with the problem by combining the uniaxial compaction tests, texture analysis and mathematical modelling. We demonstrated the Johanson compressibility factor obtained at uniaxial compression conditions can be used successfully to predict the ribbon density at different conditions of RC. Texture analysis was used to design technology transfer and scale up of the process and also as a tool to determine ribbon and granulate non-uniformity. Employing the described approaches can facilitate the adoption of RC as a granulation technology and can help minimize batch to batch variability or process fluctuation during continuous manufacturing.

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RHEOLOGICAL PROPERTIES OF PHARMACEUTICAL MIXTURES FOR ORALLY DISINTEGRATING TABLETS AND THEIR EFFECT ON FINAL TABLET PROPERTIES

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The article deals with the analysis and assessment of the rheological properties of pharmaceutical mixtures intended for the production of orally dispersible tablets (ODT).

ODTs are specifically designed for a group of patients who have problems using drugs in the form of tablets. Three commercially available co-processed mixtures Ludiflash®, Parteck®, and Prosolv® were analyzed separately and in a 1:1 ratio with the antipyretic drug Paracetamol. The examined samples were subjected to compressibility tests and shear tests on a Freeman FT4 rheometer. The flow properties of the powder mixtures were characterized using Pharmacopoeia methods. ODT tablets were created and analyzed from the powder mixtures. The addition of the drug to the co-processed mixtures resulted in higher compressibility, cohesion, and a decrease in the value of the flow function parameter, but also affected the properties of the created ODT tablets.

Acknowledgments:

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SYNTHESIS OF NEW POTENTIAL DRUGS AGAINST ALZHEIMER'S DISEASE, THEIR CHARACTERIZATION AND DISSOLUTION BEHAVIOUR

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A new report from the WHO shows that one billion people are influenced by neurological disorders worldwide. Neurological disorders affect people in all countries, no matter of age, sex, education or income.

Alzheimer's disease (AD) is a neurodegenerative disorder characterized by cognitive dysfunction and dementia. Current estimates suggest that around 50 million people are affected by this disease. Unfortunately, drugs for AD and its progression have not yet been discovered. There are several approaches in the symptomatic treatment of AD. One of them is the use of the cholinesterase inhibitors (acetylcholinesterase and butyrylcholinesterase), which have a number of side effects. Therefore, a development of new and less toxic substances is of critical importance.

A family of new compounds as potential AD drugs were prepared by six-step synthesis (figure 1). A biological activity assay was performed and *in vitro* behaviour of selected compounds was studied. Some substances displayed remarkable biological activity and became a subject of interest for further extensive testing.

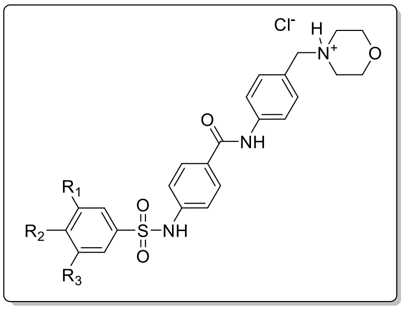

Figure 1 General structure of new potential drugs against AD.

MOLECULARLY IMPRINTED POLYMERS FOR SPE OF BIOLOGICALLY ACTIVE COMPOUND THYMOL

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Molecularly imprinted polymers (MIP) are often used as the stationary phases for solid phase extraction (SPE). MIPs dispose of various advantageous properties compared to conventional stationary phases (e.g., silica gel). The most significant advantage of MIPs is indisputably their selectivity towards analytes. The high selectivity of MIPs is determined by the preparation process in which the analyte is used as a template, i.e. the imprinted molecule. Subsequently, after washing the template out of the structure, particular binding sites, cavities, are created in the polymer structure. Moreover, MIPs prepared for the SPE process can be potentially used in other applications, such as chromatography, chemical sensors, or in drug targeting.

The key steps for the successful preparation of MIP with excellent properties are: i) the synthesis of the polymer itself and ii) the process of extracting the template molecule from the polymer in a sufficient quantity. After the successful preparation of MIP with thymol as a template molecule, we focused on the second step, the extraction. Various methods were suggested (shaking, mixing at various temperatures, Soxhlet extraction) as well as various solvents (methanol, isopropyl alcohol, diethyl ether) to evaluate the optimal extraction conditions. The extraction step proved to be quite robust. The chosen solvents as well as the extraction method and temperature did not appear to be highly critical factors (extraction yield at least 50% in all cases). Nevertheless, some of the methods were less suitable due to the degradation of the polymer particles during the extraction process (particularly mixing). MIP with selective cavities towards thymol was used in the model SPE process, where the solutions of thymol were applied to the columns filled with MIP as a stationary phase. The efficiency of thymol separation from the applied samples was in the range of 50 – 95% depending on the conditions of the SPE process showing the good potential of prepared MIP for further applications.

MATHEMATICAL MODEL OF PREDICTION OF MEAN PARTICLE SIZE OF GRANULATE

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Granulation is a size-enlarging process and plays an important role in the preparation of fine fractional powders into granules of desired properties. By adjusting the flow properties of the primary mixtures, the required flow properties of granules can be achieved and thus ensure a problem-free tableting process. The aim of this work was to create a mathematical model for predicting the D50 of granules created at different process parameters in a granulator patented by UPI.

Granules were produced by using four different impeller speeds, three wet massing times and different amounts of added granulation liquid (L/S ratio). A high-shear batch granulator was used to modify the flow properties of primary powder. The granulation liquid was sprayed into the granulator chamber. The experiments were performed at L/S ratios of 0.66 - 1.21. Large agglomerates and fine particles were removed by sieve analysis. The granule size was determined by dynamic image analysis.

The created mathematical model takes into account the significance of individual parameters on the D50 of the produced granules. On the basis of which the criteria were selected, which were used to calculate the theoretical D50 of granulates.

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BINDING CHARACTERISTICS OF MULTIMODAL ADSORBENTS: EFFECT OF SALT AND pH

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In the last four decades, antibodies experience an increasing focus of the pharmaceutical industry. Their high specificity against antigens is a factor, which makes them irreplaceable in the therapy of various diseases. Antibodies or immunoglobulins are widely used in the treatment of cancer, Crohn's disease, rheumatoid arthritis, and many other autoimmune diseases.

Nowadays, most of the costs of antibodies manufacturing are focused to the downstream section. A typical layout for the separation and purification of therapeutical antibodies includes, except for centrifugation and filtration, a variety of chromatographic steps, such as affinity, ion-exchange and hydrophobic chromatography. Multimodal adsorbents are novel types of chromatographic resins which provide more than one type of interaction with protein. Their implementation in the downstream section could reduce the number of chromatographic steps or improve the economic efficiency of purification, as they can be used in wide range of pH and salt concentrations.

This work was devoted to the investigation of the impact of different conditions on binding characteristics of multimodal adsorbents. Batch adsorption experiments with Capto adhere, Capto MMC, Toyopearl MX-Trp-650M and CHT Type 1 were conducted. As feed, solutions of polyclonal and monoclonal antibodies were used. The feed solutions were composed of monomer form and aggregates of antibodies. The main investigated parameters were the pH of the buffer, and the presence of two salt types in different concentrations. The cation-exchanger Toyopearl MX-Trp-650M and CHT Type 1 showed almost constant static binding capacity (SBC) in the pH range of 3.2 to 7. For Capto MMC, the highest SBC was observed for buffer with pH 5-6 and the SBC for Capto adhere significantly increased with increasing pH from 6 to 8.

The binding capacity of Toyopearl MX-Trp-650M in buffer with pH 4 increased from 100 mg/g to 140 mg/g after the addition of NaCl at 100mM concentration. A similar trend was observed for the second cation-exchanger Capto MMC, which SBC increased from 80 mg/g in buffer with pH 4 and without salt to 100 mg/g after 150mM ammonium sulphate addiction. On the contrary, increasing salt concentration resulted in a decrease in the binding capacity for Capto adhere in buffer with pH 7.

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EXPECTED AND UNEXPECTED IMPURITIES IN THE PRODUCTION OF CHOSEN PROSTAGLANDIN ANALOGUES AND THEIR INTERMEDIATES

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Impurities in the production of APIs can generally be divided into several categories (organic, inorganic, residual solvents and genotoxic impurities), where their source can be starting raw materials, reagents, API instability - degradation, non-specific impurities, but mainly they are impurities from the own chemical production process, i.e. by-products of chemical reactions-which we focus on.

Knowledge of the production process of not only prostaglandins is demonstrated, among other things, by knowledge (identification and isolation, or targeted synthesis) of process impurities. The manufacturer then proves the absence of identified impurities in the production intermediates or in the final product as part of the audit.

The production of synthetic analogues of prostaglandins is characterized by a number of impurities originating from the chemical production process. The key substance for production is the optical purity of the starting Corey lactone diol. It can be racemic for some applications (e.g. racemic Cloprostenol), or it must be so-called optically pure (e.g. Bimatoprost). The following several stages of production bring a whole range of expected impurities, stemming from the essence of the chemical reactions carried out. Unexpected and often undescribed impurities are a very interesting phenomenon. Their isolation, identification and possible targeted synthesis is always a challenge. An example of typical impurities for typical member of prostaglandin family Bimatoprost is shown in Figure 1.

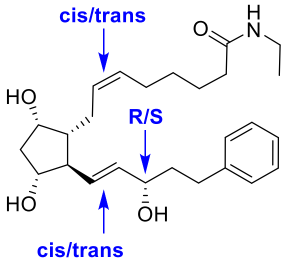

Figure 1: Typical locations of impurity formation in prostaglandin compounds shown on Bimatoprost structure.

In our practice, we have dealt with impurities of some prostaglandin analogues (alfaprostol, tafluprost) and examples of typical and unexpected impurities will be discussed.

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STUDIUM BIOLOGICKÝCH AKTIVIT DERIVÁTŮ BETULONOVÉ A PLATANOVÉ KYSELINY

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Vývoj nových antimikrobiálních a cytotoxických látek odvozených od kyselin majících triterpenoidní základ spadá do problematiky testování nových biologicky aktivních látek. Použitými výchozími kyselinami pro syntézu derivátů byly betulonová a platanová kyselina. Stěžejním krokem syntetické části byla reakce triterpenoidních kyselin s hydrochloridem hydroxylaminu v suchém pyridinu spolu s ethanolem zahřívaných pod refluxem, kterou bylo dosaženo vzniku oximových derivátů. Tyto deriváty včetně dalších syntetizovaných produktů v podobě oximesterových derivátů byly testovány na antibakteriální a cytotoxickou aktivitu. Antibakteriální aktivita byla stanovena proti kmenům modelových patogenních bakterií: Gram-pozitivních *Staphylococcus aureus* a *Enterococcus faecalis* a Gram-negativních *Escherichia coli* a *Pseudomonas aeruginosa*. Testování bylo provedeno diskovou a diluční metodou a resazurinovým testem. Cytotoxická aktivita byla testována na lidských buněčných liniích HepG2 (lidské nádorové jaterní buňky) a HEK 293T (nenádorové lidské embryonální ledvinové buňky). Cytotoxicita byla stanovena pomocí systému Real-Time Cell Analysis Dual Purpose (RTCA DP) (xCELLigence®) a resazurinovým testem.

Poděkování: Práce je podpořena projektem IGA A2_FPBT_2023_026

CORTICOSTEROID-LOADED PLGA NANOSPHERES FOR TREATMENT OF CHRONIC INFLAMMATION

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Corticosteroids are highly effective anti-inflammatory drugs with wide therapeutic use. Unfortunately, corticosteroid therapy is associated with severe side effects.[1] For safer and more effective anti-inflammatory therapy we tried to load corticosteroids into PLGA nanospheres (NSs) with predominant distribution into macrophages, key players in the development of inflammation.[2] Such formulations could be effectively employed in therapy of non-alcoholic steatohepatitis - chronic liver inflammation.[3] Using the nanoprecipitation method we prepared dexamethasone acetate-loaded PLGA NSs. The formulations were prepared in the size range 100-300 nm, which was proven as macrophage attractive, with maximum encapsulation efficiency about 20% determined by HPLC. Using the macrophage cell lines such as murine bone marrow macrophages and human macrophages (differentiated THP-1 cells) we observed effective reduction of the pro-inflammatory cytokines levels e.g. TNF-α and IL-1β by our NSs. Experiments were performed on lipopolysaccharide-induced inflammation model and no signs of cytotoxicity were observed. Furthermore, we tested our NSs labelled with fluorescent dye on in vivo models for accumulation studies. We observed fluorescence intensity of prepared NSs by IVIS Imaging System and the spectral cell analyser. We were able to verify specific delivery of prepared NSs into liver and preferential accumulation in proinflammatory macrophages.

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PREPARATION OF CFTR MODULATOR INTERMEDIATES

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Mutation of the CFTR gene causes the defective CFTR protein to fail to fold correctly, preventing it from leaving the endoplasmic reticulum and migrating to the cell surface, which causes serious health problems such as cystic fibrosis. CFTR modulators are used to modulate the function of defective CFTR protein. As a result, the substance increases CFTR ion channels' production and the total number of receptors on the cell membrane available for ion and fluid transport. There are two types of modulators - potentiators and correctors. Tezacaftor was chosen as the CFTR modulator belonging to the group of correctors. This work is focused on optimizing individual steps of Tezacaftor synthesis, especially i) methylenation of methyl homoveratrate and ii) reduction of nitrobenzene to an amine. Methylenation was performed using potassium carbonate, potassium *tert*-butoxide, and sodium hydride. The highest achieved relative concentration of product (89%) was by using sodium hydride. Several reducing agents were tested for reduction, such as sodium dithionate, tin(II) chloride, and zinc dust. The results were strongly affected by the type of reducing agent.

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TABLET MICROSTRUCTURE INFLUENCE ON DRUG RELEASE FROM TABLETS CONTAINING MATERIALS WITH DIFFERENT DEFORMABILITY

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Characteristics of used materials, the composition of the final product and process parameters have an impact on a formulation of a drug (API, active pharmaceutical ingredient) into tablets and on formulation performance, especially API release rate. To understand a formulation, knowledge of tablet microstructure is desirable. Commonly used analytical techniques, such as X-ray tomography and intrusion mercury porosimetry, are not frequently used in pharmaceutical companies due to their price and toxicity, and, therefore, there is an effort to develop a tool for fast and easy microstructure description.

In this work, we have developed an image-based method for microstructure description and applied it to a model system comprised of ibuprofen and $CaHPO_4 \cdot 2H_2O$ (API and excipient with different viscoelastic properties (deformability). The obtained parameter from image analysis, quadratic mean of equivalent circular diameter, was correlated with tablet composition, compression pressure and with API release rate.

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PREPARATION AND THE APPLICATION OF DRUG MICRO-SUSPENSIONS ON POROUS CARRIERS FOR ENHANCED DRUG DELIVERY

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Poorly soluble substances, belonging to BCS classes II and IV, constitute a significant proportion of the currently available drugs. Enhancing their bioavailability poses a major challenge, which is tackled through various strategies. One of the most widely used methods is comminution, which increases the specific surface area of the drug, thereby improving its dissolution rate and bioavailability.

There are two primary milling methods: dry and wet. When utilizing a liquid media in the milling process to create suspensions, it can be advantageous for preserving the crystalline form of the drug and preventing stability issues, as opposed to using a solution or amorphous system.

To preserve the benefits of increased specific surface area of the drug, the suspensions must be transformed into a solid form for easy and efficient use. This can be accomplished by utilizing carrier systems to control the particle size and morphology. Porous carrier-based systems offer superior surface coverage uniformity by API micro-particles, improved processability, and better powder wettability.

Our research focuses on describing the properties, performance, and preparation of systems created by loading the suspension onto the surface of the porous inorganic carrier, Neusilin® US2. This approach leads to the development of complex, ordered systems that we evaluate based on particle size, degree of carrier surface coverage, and drug release rate.

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COMBINING DIFFERENT POWDER UNIAXIAL COMPRESSION ARRANGEMENTS TO BETTER PREDICT POWDER COMPRESSIBILITY BEHAVIOUR DURING THE ROLLER COMPACTION PROCESS

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Dry granulation processes are most commonly performed with roller compaction. To find the most suitable process parameters on roller compactors involves to perform many screening and verification batches to obtain the most suitable batch of granulate for further processing (such as tableting). Most commonly, the most suitable granulate prepared this way is characterized by the unmilled intermediate called the ribbon (roller compacted compact). When such pilot studies are conducted on lab scale roller compactors the information about the intermediates of preferable batches can be characterized by their ribbon density. This ribbon density can then be used in mathematical modelling if scale-up or technology transfer is desired. The work presented minimizes the scale of pharmaceutical material processing even further as it utilizes an instrumented tablet press Gamlen D1000 with three different die sizes. The aim of this work was to show that when multiple arrangements for powder compaction simulation are utilized the compressibility of the powder (material property that is transferable to roller compaction to predict process parameters on different compactors via mathematical modelling) can be adequately utilized since the proposed experiment design helps elucidate powder densification behaviour from feeding stage (at very low pre-compaction pressures) to the compression zone where the gap between rollers is the most narrow.

TECHNOLOGY
FOR ENVIRONMENTAL PROTECTION

DIESEL EXHAUST FLUID QUALITY IMPEDANCE MEASUREMENT SYSTEM

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The possibility of measuring the quality of the diesel engine exhaust fluid (DEF, AdBlue®) used in selective catalytic reduction (SCR) systems to reduce nitrogen oxide (NO_x) emissions is discusses in this paper. There are two key motivations for quality measurement. Firstly, the quality of AdBlue® significantly influences the efficiency of SCR. Secondly, there are attepts to tamper SCR systems by replacing DEF with water. DEF quality measurement is therefore required by regulations such as California Air Resources Board (CARB) or European emission standards (EURO 1-6). The quality of AdBlue® is affected by factors such as storage conditions, contamination and degradation. The results of AdBlue® quality measurements can be used to ensure optimal engine performance and minimize environmental impact. Different types of systems based on acoustic wave-based sensors, optical sensors, and others are used for measuring AdBlue® quality in vehicle. Impedance spectroscopy is a non-destructive technique used to study the electrical properties of materials over a wide range of frequencies. The technique has a high sensitivity and can provide valuable information about the properties of the different materials. The paper explores the impedance spectroscopy for measuring AdBlue® quality and the results demonstrate the possibility of using this method.

CORRELATIVE SPECTRO-MICROSCOPY FOR IDENTIFICATION AND CHARACTERIZATION OF MICROPLASTICS IN WASTEWATER AND DRINKING WATER

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Plastic has become the most common material in our life during the last decades. However, the increased consumption of plastics has resulted in their global presence and accumulation in the environment. The prevalence of plastic tends to be the most concern for the potential risks to human health. Moreover, one of the major problems is the degradation of plastic into microplastic (MPs). From this point of view, the identification and characterization of MPs are still a challenge.

Traditionally, MP identification includes visual assessment and chemical confirmation. Microscopy is the most used way for the visualization of MP morphology. The primary advantages of this technique are simplicity and rapidity, but there is a high possibility of false positive data. Spectroscopy is utilized for the confirmation of MP chemical composition. The most common method is FTIR spectroscopy as a non-destructive analysis, which reduces false negative data and can detect MPs down to 10 µm in size. Nevertheless, FTIR is time-consuming and covers a limited area for the selected wavenumbers. Alternatively, Raman spectroscopy has been widely used for the characterization of MPs. This analysis can identify MPs down to 1 µm. Besides, as a non-destructive and non-contact method, Raman spectroscopy provides a possibility for the investigation of the same sample by different techniques. However, the main disadvantage of this analysis is the limitation of spatial resolution.

Herein, we propose correlative spectro-microscopy as a fast and reliable method for the identification and characterization of MPs. This approach combines the strongest points of microscopy (SEM-EDS) to provide excellent information about morphology and element-specific composition while Raman spectroscopy allows to identify a fingerprint of chemical compositions.

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AMMONIA ABATEMENT FROM LIVESTOCK BUILDINGS USING ADVANCED OXIDATION PROCESSES

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The feasibility of using advanced oxidation processes (AOPs) for abatement of ammonia from livestock buildings was examined in a series of pilot plant experiments. In this study, all the experiments were conducted in a two-step unit containing a dry photolytic reactor ($UV_{185}/UV_{254}/O_3$) and a photochemical scrubber (UV_{254}/H_2O_2). The unit efficiency was tested for two initial ammonia concentrations (20 and 35 ppmv) and three different air flows (150, 300 and 450 $m^3 \cdot h^{-1}$). While the first step removes mainly organic pollutants that are often present together with ammonia in the air and ammonia only partially, the second step removes around 90 % of ammonia emissions even at the highest flow rate of 450 $m^3 \cdot h^{-1}$. Absorbed ammonia in the aqueous phase can be effectively removed without adjusting the pH (i.e. without the addition of other additives) using UV and ozone. Complete removal of ammonia was achieved after 15 hours of irradiation. In order to assess the price efficiency of the suggested technology and to be able to compare it with other methods the figures-of-merit were determined. The price needed for lowering ammonia emission by one order of magnitude is 0.002 € per cubic meter of treated air at the highest flow rate of 450 $m^3 \cdot h^{-1}$ and for initial ammonia concentrations of 20 ppmv. These findings demonstrate that AOPs are a promising method for ammonia abatement from livestock buildings which are rarely using any waste air treatment method.

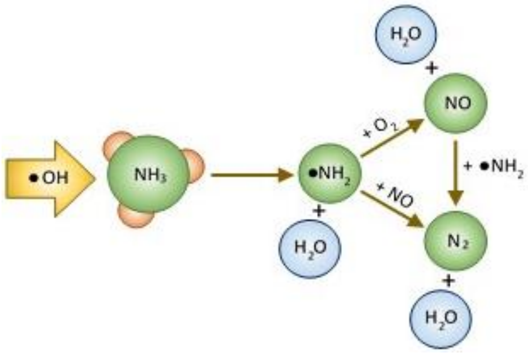

Fig. 1. Scheme of mechanism of ammonia degradation

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RECENT PROGRESS IN DIRECT NO DECOMPOSITON OVER K/Co-BASED MIXED OXIDES

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Nitric oxide (NO) is one of the oxides from a group known as NO_x (NO, NO_2), which are produced by anthropogenic activities and represent serious environmental problem. Most of the waste gases consist of 95% of NO. Direct decomposition of NO to N_2 and O_2 can be an effective method for abatement of NO emissions. Direct NO decomposition is a spin-forbidden reaction with high activation energy (364 kJ/mol). Therefore, the reaction takes place at high temperatures (1100-1200 °C) or the catalyst has to be used to increase reaction rate. Although many catalysts have been already tested (noble metals, metal oxides, zeolites), the development of active and stable catalyst still remains a challenging subject of basic research [1].
The aim of this presentation is to summarize the so far obtained results of our research focused on the direct NO decompositon over K-modified Co-based mixed oxides. In last years, we have systematically studied the effect of preparation parameters (calcination temperature and time [2], type and amount of alkali metal precursor, preparation method [3]) on the catalyst activity, stability and selectivity in inert gas and in the presence of co-existing gases (O_2, H_2O, CO_2, SO_2). Partial substitution of Co by Mg [4], Zn [5] and Mn was also performed. Various characterization methods (AAS, XRD, S_{BET}, SEM, TEM, XPS, TPD-CO_2, TPR-H_2, SR-TAD) were used for determination of physico-chemical properties. Moreover, using TPD-NO, in-situ FTIR and transient kinetic state experiments, the surface intermediates were studied and reaction mechanism of direct NO decomposition over K/Co-based mixed oxides was proposed [6].
From obtained results, it can be concluded that the presence of K, which affects catalysts basicity, is essential for catalytic activity, since the non-promoted catalysts were totally inactive, and so is the presence of Co. On the other hand, Mn and Mg play the role as structural promoters, affect the surface area and ensure the catalyst stability.

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TWO STAGE PYROLYSIS/SPLIT PRODUCT GASIFICATION OF REFUSED-DERIVED FUEL: PRODUCT DISTRIBUTION

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Numerous studies have shown the detrimental effect of waste on the environment and on plants, animals and humans. However, simply renouncing the production of waste is not possible, as it would mean a reduction in nutrition and the quality of life of people. Consequently, waste production continues, and procedures of the waste processing should be developed. Part of non-recyclable municipal waste can be used as a source of energy or as a raw material. For this purpose, it is necessary to separate refuse-derived fuel (RDF) from municipal solid waste and subject it to heat treatment. In this study, a real RDF sample was thermally decomposed in a laboratory two-stage reactor. In the first reactor stage, pyrolysis of RDF took place, and subsequently, in the second step, the pyrolysis products were gasified using a substoichiometric amount of air. In selected experiments, RDF gasification was carried out in the presence of tar-cracking catalyst. The effect of reaction conditions and catalyst presence on the raw material conversion, gasification products distribution, producer gas composition and quality were monitored. Also, the fate of contaminants, sulfur and chlorine, present in RDF was investigated. By increasing the equivalence (oxidant-to-feed mass) ratio, the amount of solid product (gasification char) was decreased while that of liquid and gaseous products increased. After pyrolysis, about 75% of sulfur and more than 90% of chlorine originally present in RDF remained in the solid phase. However, pyrolysis char gasification caused volatilization of contaminants thus considerably reducing their content in the solid product. The increase in equivalence ratio caused a decrease in producer gas lower heating value, while an optimum equivalence ratio ($ER = 0.19$) was observed regarding the hydrogen content in producer gas. Tar reduction in the producer gas was potentiated by the equivalence ratio increase; the catalyst presence was less pronounced.

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STUDY OF THE KINETICS OF GLYPHOSATE SORPTION ON GRANULAR ACTIVATED CARBON

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Introduction

Micropollutants (MP) are persistent substances added to water due to human activity, and whose concentration is higher than the normal "natural" background. Although their low concentration (10^{-9} to 10^{-6}g l^{-1}), they can be a potential threat to humanity, especially in the long term. One of the important MP is glyphosate (GLY), a broad-spectrum herbicide widely used in the eradication of annual and perennial weeds. Despite its positive soil-binding properties, GLY could accumulate in surface water. Thus, the necessity of efficient removal of GLY from wastewater raises the need for separation techniques such as GLY adsorption on granular activated carbon (GAC). Our study is aimed at studying the repeated adsorption of GLY on fresh/aged GAC in order to simulate the process of GLY removal procedures and to evaluate the long-term performance of GAC.

Experimental

Granular activated carbon (Hydraffin CC, from coconut shells) was purchased from DONAU-CARBON and characterized by N_2 sorption (BET) and TGA/DSC methods.

Sorption of GLY onto GAC was first studied using BATCH experiments performed in 500 ml glass flasks equipped with magnetic stirring. The flasks were filled with 5 g of GAC in deionized water. The experiments consisted in adding a defined amount of GLY in an aqueous solution flasks, and the GLY concentration was followed for 24hr by ion chromatography. Then this procedure was repeated and the original GAC was left in the flask. The initial concentration of GLY was varied to investigate the effect of concentration on adsorption kinetics.

Furthermore, two types of flow experiments were performed in a fixed-bed filtration unit containing 100 g of fresh GAC or aged GAC that had been exposed for 5 months to wastewater (50-20 mg L^{-1} COD). In these experiments, a solution of 50 µg/L GLY was fed into the system and samples of the permeate were taken at 30 min intervals.

Results and discussion

Results from BATCH experiments (over 90 experimental runs) were processed by non-linear regression in order to describe the data by different kinetic models. The obtained kinetic parameters were applied in a dynamic model of a GAC fixed-bed filtration unit. A satisfactory agreement was found between the experiments from the flow experiments and the predictions based on the data obtained from the BATCH experiments.

ENVIRONMENTALLY ACCEPTABLE LUBRICANTS for STERN TUBES APPLICATION

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Legislative restrictions exist on using mineral oils for loss lubrication of marine propellers. Vessels larger than 24 m must use environmentally acceptable lubricants for the stern tube lubrication. Emphasis on developing renewable, biodegradable, and environmentally acceptable lubricants has resulted in the widespread use of natural oils and fats. Synthetic oils are also promising candidates as the base fluid for such a class of lubricants because of their excellent lubricity, biodegradability, viscosity-temperature characteristics, and low volatility. However, the suitability of the vegetable oils for a specific application either needs chemical modification or may be used as it is with an additive blending route to get the base stocks as per specifications for a particular end-use application. A key question is finding a functionally suitable and economically acceptable substitute for mineral lubricants. The answer will make it possible to fundamentally limit the impact of international shipping on the marine ecosystem.

This work presents the results of an experimental study of four types of base fluids and the influence of seawater on their properties. The results show that base fluids based on vegetable oils have a high viscosity index, i.e., their viscosity changes slightly with temperature. However, at the same time, they contain a relatively large amount of free fatty acids, which promote corrosion (high total acid number). The viscosity of saturated and unsaturated synthetic esters is more temperature dependent. However, their total acid number is significantly lower, making them suitable candidates for these applications.

The work was supported by the project TO01000250 Novel Routes to Environmentally Acceptable Lubricants-REAL benefits from a grant from Iceland, Liechtenstein, and Norway through the EEA Grants and the TACR within the KAPPA Programme.

CATALYTIC WET AIR OXIDATION OF PHENOL WASTE WATER USING THE COMNFE CATALYST IN CONTINUOUS FLOW QUARTER-SCALE REACTOR AND ITS POTENTIAL USE IN INDUSTRIAL SEGMENT.

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Hydrotalcite-like materials (LDH´s) are recognised as an excellent material for catalytic application. These materials were applied in wide range of applications, such as catalytic wet air oxidation process (CWAO) for a waste water treatment. During the oxidation pathway of high molecular weight organic compounds, a toxic intermediate phenol may occur. To evaluate the CWAO water treatment consisting of phenol, our research tested the double-layered hydrotalcite (LDH’s) CoMnFe catalyst for its potential application in industrial scale. The CoMnFe catalyst was prepared by co-precipitation method with molar ratio 4:1:1 and tested for its chemical composition (ICP-OES) and textural properties using XRD and N_2-physisorption. The quarter-scale unit was used to test the activity of the catalyst in continuous-flow arrangement using the model water consisting of 900 ppm of phenol, where the phenol concentration was analyzed by HPLC and GC-MS. Our results showed, that the catalyst CoMnFe was most active during the first 24 h and after regeneration, where the concentration of phenol significantly decreased. However, this experiment also proposes the dependency of the operating conditions, which are very specific for CWAO process, especially the temperature.