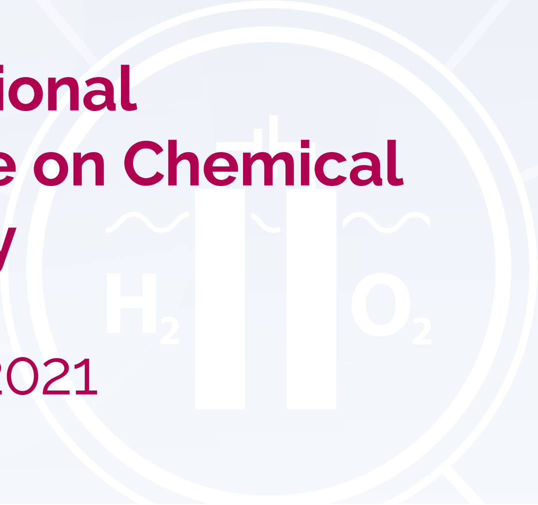
ICCT

INTERNATIONAL CONFERENCE
ON CHEMICAL TECHNOLOGY

8th International Conference on Chemical Technology

May 3 – 5, 2021



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ICCT 2021 | Scientific program, LECTURES

MONDAY, MAY 3

8:45–9:00	*Jaromír Lederer, Jaromír Lubojacký* **Opening**

Moderator: Jaromír Lederer (ORLEN UniCRE)

9:00–9:25	*KL1 – Tomáš Herink (ORLEN Unipetrol)* **New investment in Unipetrol RPA – Polyethylene III**
9:30–9:50	*OP/SL1 – Hugo Kittel (UCT in Prague)* **Utilization of synergies between oil refineries and bio-refineries as an important factor in their further development**
9:55–10:15	*OP/SL2 – Adam Karaba (UCT in Prague)* **Co-pyrolysis of Fischer-Tropsch wax vacuum residue with hydrocracking product**
10:20–10:40	*OP/SL3 – Martina Slezáčková (VÚRUP, Bratislava)* **Partial hydrogenation of double bonds in polyunsaturated fatty acid methylesters**
10:45–11:05	*OP/SL4 – Jáchym Mück (University of Pardubice)* **Transformation of ethanol to higher alcohols by transition metal promoted Mg-Al mixed oxides in flow reactor**
11:05–11:30	*Break*

Moderator: Petr Zámostný (UCT in Prague)

11:30–11:50	*OT/SL5 – Martin Veselý (UCT in Prague)* **Autogenous formation of gold-phosphorene nanohybrids and their application in catalytic purification of wastewater**
11:55–12:15	*OT/SL6 – Roman Valeš (UCT in Prague)* **The effect of water and substituents of aromatic ring on its hydrogenation over a cobalt catalyst**
12:20–12:40	*OT/SL7 – Maria Kotova (UCT in Prague)* **Synthesis of new ruthenium complexes and their use as catalysts in hydrogenation of diene compounds**
12:45–13:05	*OT/SL8 – Kateřina Zítová (UCT in Prague)* **Preparation of α-terpineol and perillyl alcohol using zeolite beta**
13:10–14:00	*Break*

Moderator: Bohumil Kratochvíl (UCT in Prague)

14:00–14:20	*OT/SL9 – Lenka Hašková (UCT in Prague)* **Solvent effects in aldol condensation – production of important fragrance**
14:25–14:45	*ME/SL10 – Jan Smolík (University of Pardubice)* **Direct laser writing on the surface of $PbO-Bi_2O_3-Ga_2O_3$ glasses**
14:50–15:10	*ME/SL11 – José Miguel Hidalgo Herrador (Orlen UniCRE)* **Phonolite. An available, natural czech resource for producing novel valuable materials**
15:15–15:35	*ME/SL12 – Monika Chládková (University of Pardubice)* **Chemical structure of $MoO_3-P_2O_5$ binary glasses**
15:40–16:00	*Break*

Moderator: Bohumil Kratochvíl (UCT in Prague)

16:00–16:25	*KL2 – Ivan Souček (SCHP ČR)* **Decarbonisation of the chemical industry in the light of Green Deal requirements**
16:30–16:50	*ME/SL13 – Klára Kobetičová (CTU in Prague)* **Chitin-caffeine models in biocidal wood coatings**
16:55–17:15	*ME/SL14 – Martin Hájek (University of Pardubice)* **The influence of long-term aging on structure of Mg-Al mixed oxides and catalytic activity of aldol condensation**
17:20–17:40	*ME/SL15 – Jana Sklenářová (CTU in Prague)* **Controlled triboelectrification of dust particles as a promising method for the improvement of electrodynamic cleaning systems**
17:45	Closing, Invitation to poster session

18:00–19:00	**POSTER SESSION**

TUESDAY, MAY 4

Moderator: Bohumil Kratochvíl (UCT in Prague)

9:00–9:25	*KL3 – Ladislav Cvak (TCI Opava)* **Czech pharmaceutical industry – recent history and actual view**
9:30–9:50	*SP/SL16 – Pavlína Komínová (UCT in Prague)* **Rheological properties of powder mixtures as a factor of hard-gelatin capsule filling performance**
9:55–10:15	*SP/SL17 – Simona Römerová (UCT in Prague)* **Tablet microstructure evolution during the compaction process**
10:20–10:40	*SP/SL18 – Eva Petříková (UCT in Prague)* **Application of Hansen solubility parameters in pharmaceutical industry**
10:45–11:05	*SP/SL19 – Aneta Vovesná (UCT in Prague)* **Ceramide liposomes: Formulation of stratum corneum lipids for skin barrier recovery**
11:05–11:30	*Break*

Moderator: Bohumil Kratochvíl (UCT in Prague)

11:30–11:50	*SP/SL20 – Kristýna Dvořáková (UCT in Prague)* **Morpholine derivatives: Novel substances for modulating the permeability of the skin barrier**
11:55–12:15	*SP/SL21 – Michaela Slámová (UCT in Prague)* **Improving dissolution rate of poorly soluble drugs by milling and co-milling technique**
12:20–12:40	*SP/SL22 – Jiří Barek (Charles University, Prague)* **Possibilies and limitations of electroanalytical methods in pharmaceutical analysis**
12:45–13:05	*SP/SL23 – Adéla Bártová (UPOL, Olomouc)* **Batch or continuous crystallization & their effect on physicochemical properties of solid phase**
13:10–14:00	*přestávka*

Moderator: Ivan Souček (SCHP ČR)

14:00–14:20	*EC/SL24 - Ivan Souček (SCHP ČR)* **Current trends in the chemical industry in the Czech Republic**
14:25–14:45	*EC/SL25 – Kristián Hanus (Slovnaft)* **Techno-economic optimization of steam cracker's steam network**
14:50–15:10	*EC/SL26 – Zuzana Dvořáková (UCT in Prague)* **Digital well-being for highly skilled staff**
15:15–15:35	*EC/SL27 – Marek Botek (UCT in Prague)* **Personal and transversal competencies in bio-based economy**
15:40–16:00	*přestávka*

Moderator: Ivan Souček (SCHP ČR)

16:00–16:25	*KL4 – David Kubička (UCT in Prague)* **Green chemistry – the case of renewables**
16:30–16:50	*EC/SL28 – Lenka Branská (University of Pardubice)* **Attitudes of consumers to household waste sorting**
16:55–17:15	*EC/SL29 - Dalibor Vytlačil (UCT in Prague)* **System model of maintenance dynamics**
17:20–17:40	*AP/SL30 – Jiří Kroužek (Dekonta)* **Innovative technology PLASMICAT for hazardous air treatment**
17:45	Closing, Invitation to poster session

18:00–19:00	**POSTER SESSION**

WEDNESDAY, MAY 5

Moderator: Petra Patáková, Barbora Branská (UCT in Prague)

9:00–9:25	*KL5 – Kamil Wichterle (VSB TU, Ostrava)* **Carbon balance in nature and in technologies**
9:30–9:50	*BI/SL31 – Petra Patáková (UCT in Prague)* **Meat from Petri dish**
9:55–10:15	*BI/SL32 – Anna Miškovská (UCT in Prague)* **Biosynthesis of metal nanoparticles using vitis vinifera extract and their antimicrobial activity**
10:20–10:40	*BI/SL33 – Markéta Husáková (UCT in Prague)* **Genus monascus and its secondary metabolites**
10:45–11:05	*BI/SL34 – Petra Kašparová (UCT in Prague)* **Antimicrobial and antivirulence activity of pterostilbene, methoxylated derivative of resveratrol**
11:05–11:30	*Break*

Moderator: Petra Patáková, Barbora Branská (UCT in Prague)

11:30–11:50	*BI/SL35 – Michaela Rollová (UCT in Prague)* **Effects of Vitis vinifera extracts on representatives of gastrointestinal tract-associated microorganisms**
11:55–12:15	*BI/SL36 – Dominik Maršík (UCT in Prague)* **Antimicrobial activity of chitosan nanoparticles against Pseudomonas aeruginosa**
12:20–12:40	*BI/SL37 – Veronika Kazimírová (STU in Bratislava)* **Production of lipoxygenase pathway enzymes by recombinant E. coli**
12:45–13:05	*KL6 – Ladislav Novák (SUSCHEM CZ)* **European Green politics Green Deal – the largest set of agendas in the existence of EU**
13:10–14:00	*přestávka*

Moderator: Antonín Kuta (UCT in Prague)

14:00–14:20	*PC/SL38 – Milan Králík (STU in Bratislava)* **Deacidification and preservation of cellulosic objects of cultural heritage**
14:25–14:45	*PC/SL39 – Milan Libánský (Metrohm Česká republika)* **It´s all made of plastic – the efficiency boost for polymer industry with vibration spectroscopy**
14:50–15:10	*PC/SL40 – Patrik Bouřa (UCT in Prague)* **Preparation of micro-cellular biopolymeric foams by thermally induced phase separation (tips)**
15:15–15:35	*WT/SL41 – Pavol Rak (UCT in Prague)* **Pozolan activity of calcined clays and other pozzolans using the Frattini test**
15:40–16:00	*přestávka*

Moderator: Antonín Kuta (UCT in Prague)

16:00–16:25	*WT/SL42 – Vít Nýdrle (University of Pardubice)* **Reductive degradation of m-trifluoromethylaniline and flufenamic acid from model wastewater**
16:30–16:50	*WT/SL43 – Simon Jantač (UCT in Prague)* **Triboelectric separation of plastic waste and utilization of external electric field to increase its efficiency**
16:55	Closing

main partner

partner

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Sekce Cestovní mapa vývoje chemického průmyslu v ČR ve světle evropské politiky Green Deal

Moderator: Ladislav Novák (SUSCHEM CZ)

14:00–14:15	*Ondřej Knotek (Evropský parlament)* **EGD a související legislativa, pohled MEP**
14:15–14:30	*Vladislav Smrž (Ministerstvo životního prostředí)* **Chemická strategie - vliv na vývoj legislativy (EU a ČR)**
14:30–14:45	*Pavlína Kulhánková (Ministerstvo průmyslu a obchodu)* **EGD z pohledu MPO**
14:45–15:00	*Jiří Reiss (Česká TP PLASTY)* **Green Deal a chemická recyklace plastů**
15:00–15:15	*Alena Krejčová (Svaz chemického průmyslu ČR)* **Implementace Strategie pro udržitelnost v oblasti chemických látek v roce 2021**
15:15–15:30	*Petr Pracna (Technologické centrum AV ČR)* **Nové příležitosti pro financování relevantních aktivit v Horizontu Evropa**
15:30–15:45	*Martin Šilhan (SUSCHEM CZ)* **Cestovní mapa SUSCHEM CZ**

KL:	*Keynote lecture (25 min)*
SL:	*Short lecture (20 min)*
P:	*Poster*

SL: Topics / Sessions

OP:	Oil, Petrochemicals, Biofuels
ME:	Materials engineering
OT:	Organic technology
PC:	Polymers, composites
WT:	Waste treatment, water protection
EC:	Economics of chemical industry
SP:	Synthesis and production of drugs
AP:	Air protection, technologies for soil decontamination
BI:	Biotechnology and biorefinery

ICCT 2021 | Scientific program, POSTERS

Poster session schedule

Monday, May 3, 18:00–19:00

Tuesday, May 4, 18:00–19:00

We ask the authors of the poster presentations to be present at the live chat during the poster session for any questions from the participants.

Oil, Petrochemicals, Biofuels

P1	*Miroslava Mališová (STU in Bratislava)* **Heterogeneous transesterification of camelina sativa catalysed by potassium impregnated Mg/Al mixed oxides to prepare biodiesel**
P2	*Božena Vasilkovová (STU in Bratislava)* **Combined thermal and catalytic cracking of waste plastics in the presence of clinoptilolite**
P3	*Miroslav Variny (STU in Bratislava)* **Modeling oxygen production via cryogenic air separation**
P4	*Petr Jíša (Orlen UniCRE)* **Alternative usage of MSCR test for evaluation of type and content of the used polymer**
P5	*Dominik Schlehöfer (Orlen UniCRE)* **Compatibility of marine fuels containing alternative materials**
P6	*Karolína Dlasková Jaklová (Orlen UniCRE)* **Co-processing of pyrolysis products**
P7	*Héctor de Paz Carmona (Orlen UniCRE)* **Co-processing of atmospheric gas oil with furfural-acetone aldol condensation adducts**
P8	*Tomáš Cibulka (Slovnaft)* **Hydrogen production optimization in refining industry**

Gas, Coal, Fuel

P9	*Petr Seghman (CTU in Prague)* **Mutual interaction of components during membrane separation of gases**
P10	*Miroslav Variny (STU in Bratislava)* **Industrial combined heat and power plant repowering proposal**
P11	*Jan Kulas (ÚJV Řež / UCT in Prague)* **Catalytic methanization biogas using catalysts based on Ni and Ni/Co**

Materials engineering

P12	*Klára Kobetičová (CTU in Prague)* **Binding interactions of metylxanthines to beech wood**
P13	*Kateřina Strejcová (Orlen UniCRE)* **Influence of the additoin of blast furnace slag to alkali-activated mixtures based on natural zeolites**
P14	*Aleš Imramovský (University of Pardubice)* **Substituted diphenylamino styryl benzenes as promissive materials with tunable intenzive solid state fluorescence – synthetic approach to key intermediate**
P15	*Halyna Starukh (VSB TU, Ostrava)* **Precursor-reforming synthesis of mesoporous g-C_3N_4 nanosheets for photocatalytic destruction of organic dye and pharmaceuticals**
P16	*Halyna Starukh (VSB TU, Ostrava)* **Tio2-LDH nanocomposites for organic dye removal from aqueous media by adsorption and photocatalytic degradation**
P17	*Milan Olšovský (ZVS IMPEX)* **Development of ecological pyrotechnic compositions**

Organic technology

P18	*Blažej Horváth (STU in Bratislava)* **Catalytic transformations of bioethanol**
P19	*Tomáš Soták (STU in Bratislava)* **Catalytic oxidation of furfural to maleic acid in the presence of iron based catalysts**
P20	*Tomáš Soták (STU in Bratislava)* **Effect of the support on manganese carbon catalysts for oxidation of cyclohexanone by molecular oxygen**
P21	*Eliška Pilařová (University of Pardubice)* **Preparation of pseudopeptide aldehydes and vinyl sulfones as a potencional proteasome inhibitors**
P22	*Olga Gorlova (UCT in Prague)* **Selective Meerwein-Ponndorf-Verley reduction of cinnamaldehyde over Al-containing catalysts**
P23	*Roman Valeš (UCT in Prague)* **The effect of temperature and concentration of water on oxidation of dicyclohexylamine with air**

Polymers, composites

P24	*Silvie Duřpeková (Tomáš Baťa University in Zlín)* **A comparative study of different polymer matrix with photoactive pigment on thermal and antibacterial properties**
P25	*Silvie Duřpeková (Tomáš Baťa University in Zlín)* **Swelling properties and biodegradability of a new agro-hydrogel based on renewable materials for agricultural use**
P26	*Elena Hájeková (STU in Bratislava)* **Two stage catalytic cracking of HDPE and PP in the presence of natural and synthetic zeolites**
P27	*Kateřina Setničková (ICHP CAS, Prague)* **Amine-functionalized porous polymers for selective CO_2 adsorption**

Economics of chemical industry

P28	*Jan Vávra (University of Pardubice)* **Limits and barriers to product life cycle monitoring for chemicals – a case study**
P29	*Jana Košťálová (University of Pardubice)* **Green human resource management in companies of Czech chemical industry**
P30	*Michal Paták (University of Pardubice)* **Sustainable packaging innovations for cosmetic products**
P31	*Josef Košťálek (UCT in Prague)* **Identification of factors influencing oil and gas prices and their mutual correlations**
P32	*Josef Košťálek (UCT in Prague)* **Identification of factors influencing oil and gas prices and their mutual correlations**

Synthesis and production of drugs

P32	*Jana Brokešová (Charles University, Hradec Králové)* **Preparation of meloxicam interactive powder mixtures by mixing and co-milling: Surface energy and dissolution rate study**
P33	*Aleš Imramovský (University of Pardubice)* **A stereoselective study of alfaprostol omega chain synthesis – application possibilities in the synthesis of intermediates**
P34	*Radim Bittner (UCT in Prague)* **Dissolution kinetics of commercially available tablets using an optical microscopy technique**
P35	*Jan Petr (UCT in Prague)* **Monitoring the roll compaction process via ribbon stiffness measurement**
P36	*Nikita Marinko (UCT in Prague)* **Technique of pharmaceutical powder compressibility measurement for utilization in predictive mathematical modelling of compaction processes**

Waste treatment, water protection

P37	*Lucie Šudomová (Brno University of Technology)* **PET-G as a PET contaminant**
P38	*Lukáš Krátký (CTU in Prague)* **Modelling particle size characteristics and specific energy demand for knife-milled beech chips at different moistures**
P39	*Amer Inayat (VSB-TU Ostrava)* **Resource recovery from waste polystyrene via thermo-catalytic depolymerization**
P40	*Klára Pulcová (UCT in Prague)* **Resistance of mixtures of Czech high temperature ash associates to alternative freezing and thawing**

Air protection, technologies for soil decontamination

P41	*Petr Praus (VSB TU, Ostrava)* **Photocatalytic decomposition of nitrous oxide over sulphur modified graphitic carbon nitride**

ABSTRACTS

LECTURES / ORAL PRESENTATIONS

KL03

CZECH PHARMACEUTICAL INDUSTRY – RECENT HISTORY AND ACTUAL VIEW

Cvak L.

TCI, Opava, Czech Republic

At the beginning, there was Spofa. The beginning means the time before the Velvet revolution in 1989, and Spofa means “Joint Pharma” (Spojená farmacie), a group of all pharma factories in former Czechoslovakia. Some drugs, mainly API used to be manufactured also in factories belonging to classical chemical industry, in companies Synthesia, Lachema and Spolana.

As soon as in 1990, all the factories and research institutes joined in Spofa became independent and they were privatized by their own way. Some of them were purchased by foreign companies (Teva, Sanofi), some stayed independent, but most of them survived up to now. Some other companies, most of them producing generic dosage forms, were established after the revolution. The result of such development is the actual state of pharma industry in Czech. There are plenty of pharma companies but bigger players, which could be denominated as Czech Pharma companies are missing.

That everything will be presented in the lecture in details.

KL05

BILANCE UHLÍKU V PŘÍRODĚ A V TECHNOLOGIÍCH

Wichterle K.

VŠB Technická univerzita Ostrava, Ostrava ČR

Vedle asi 50.10^{15}t uhlíku v karbonátových horninách, máme tu ještě několik bilionů tun uhlíku, zapojených do přírodního koloběhu v ovzduší, v rozpuštěném CO_2 a HCO_3^- v oceánech a v živé přírodě. Z tohoto cyklu se asi 40 miliard t uhlíku ročně ukládá krátkodobě v redukované formě do rostlin, humusu a usazenin, a dlouhodobými procesy do fosilních paliv. Známé zásoby fosilních paliv, asi 2,5 bilionů tun C, se za posledních 200 let značně ztenčují, v současnosti rychlostí 9 miliard tun za rok. S tím stoupá obsah CO_2 v ovzduší, současně s uvolňováním CO_2 z moře při ústupu malé doby ledové, datovaném do stejné etapy. Argument, že tím lidstvo vyvolává globální oteplení, vede k pošetilým nápadům oxid uhličitý z koloběhu odebírat. Jedinou racionální možností je však omezit spalování uhlíku. Příspěvkem tu mohou být nefosilní zdroje energie, kam přiřazujeme i energii jadernou. Podstatnou však stále bude racionalizace spotřeby fosilních paliv na elektřinu, teplo a dopravu, kde se společnost dosud smiřuje s ohromnými ztrátami. (Chemické technologie, které inovují podstatně rychleji, jsou na tom o něco lépe.) Dá se najít spoustu možností úspor, kterým bohužel těžaři fosilních paliv a producenti energie brání nízkými cenami. Současná úroveň techniky umožňuje např. při stejné účinnosti a bezpečnosti technologií bez dalších nároků na obsluhu a údržbu rozumným zmenšováním kapacit a sezónním provozem snížit zásadně nároky na energii a dopravu. Lpění na tradičních postupech vede zpravidla jen k nákladným pokusům o zmírnění některého z řady jejich nežádoucích účinků. Klíčem k budoucnosti spíše budou revoluční technická řešení. V každém případě je podstatným zachovat organický uhlík pro potřebu těch chemických procesů, ve kterých bude nezastupitelný i v prozatím vzdálené době, v níž se zdaří získávat neomezené množství energie z termojaderných elektráren, a vodík se stane levnějším a dostupnějším než uhlík.

OP/SL01

UTILIZATION OF SYNERGIES BETWEEN OIL REFINERIES AND BIO-REFINERIES AS AN IMPORTANT FACTOR IN THEIR FURTHER DEVELOPMENT

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The number of oil refineries is declining in Europa (George 2020), because petroleum products are considered as a significant GHG source. The concept of bio-refineries was developed intensively in the last decade as an alternative to oil refineries, e.g. the Task 42 of IEA (IEA 2020). Although the terms "oil refinery" and "bio-refinery" sound similar, are not. There exist big differences, however, also significant synergies as concerns feeds, capacities, technologies, products, logistic, safety, environment, potential partners, investors and CAPEX of these two concepts. Despite the fact that every oil refinery was already partially transformed into a bio-refinery processing bio-ethanol, FAME, and producing ETBE, HVO, HEFA, green propane etc., this will not be enough to meet the goals of the circular economy. It seems, that just researching, pilot-testing, scale-up, and commissioning synergies between oil and bio-refineries will be crucial for a future strategy of the oil business. Therefore, currently communicated visions of the leading oil companies and the renowned technology licensors (Hirs 2020), as well as pioneering experiences of the conversion of the oil refineries Venice (ENI_Venice 2020), Gela (ENI_Gela 2019), La Méde (Total 2020), Rodeo / San Francisco (Phillips 66 2020), Port Westward (Next Renewable Fuels 2019), etc. to a bio-refinery will be the subject of this paper.

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OP/SL02

CO-PYROLYSIS OF FISCHER-TROPSCH WAX VACUUM RESIDUE WITH HYDROCRACKING PRODUCT

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The presented study deals with the assessment of the traditional feedstock co-pyrolysis possibility with the wax fraction produced via Fischer–Tropsch (FT) synthesis. The samples of wax fraction (FT wax) coming from experimental pilot-plant Fischer–Tropsch unit plant were studied. The vacuum distillate from the hydrocracking process (HCVD) was used as the traditional feedstock. The yields of individual products and fractions from pyrolysis and co-pyrolysis of the wax fraction with traditional HCVD feedstock were measured using the laboratory micro-pyrolysis technique, which was carried out at 815 °C peak temperature and 0.2 s residence time. The experimental study showed the FT wax yields being superior in the valuable lighter olefinic products in comparison to the traditional HCVD feedstocks providing for example as much as 43 % wt. of ethylene. The mixing effects of co-pyrolysis were not significant, and the yields of most products were proportional to the FT wax content in the co-pyrolysed feedstock.

OP/SL03

PARTIAL HYDROGENATION OF DOUBLE BONDS IN POLYUNSATURATED FATTY ACID METHYLESTERS

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Some non-food oils contain a high proportion of polyunsaturated acids. This determines their oxidation stability and limited use in the production of FAME. One such raw material is oil from the plant *Camelina sativa*, L. (Crantz). The proportion of oil in the seed of camelina is in the range of 35-42 % wt. Compared to rapeseed oil, it contains the highest proportion of unsaturated linolenic acid, which causes good low-temperature properties, but also a high iodine value above 150 mg I_2/g. Its properties are more similar to linseed oil, but its thermal stability is much higher. It is necessary to technologically reduce the iodine value below the standard value of 120 mg I_2/g, while maintaining other beneficial properties to the maximum extent.

One possible solution is the partial hydrogenation of unsaturated bonds with minimal skeletal isomerization of cis-trans. Trans isomers have a higher solidification temperature than cis isomers. In the tests, we used mechanically pressed oil from the Smilovska variety degummed with citric acid, refined with bleaching clay. The second raw material was cable oil methyl ester from transesterification with sodium methanolate.

Cu-based catalysts were prepared as hydrotalcites, which were converted to mixed oxides (450 °C) by annealing. The prepared Cu mixed oxides and reduced Cu catalysts were characterized by selected adsorption and spectral methods.

The properties of the partial hydrogenation products were evaluated by measuring the refractive index, iodine value and GC (converted to methyl esters to oils) and GC-MS and evaluating the oxidation stability. Copper-based catalysts are excellent catalysts for the partial hydrogenation of olefins. Catalysts with a high dispersion of Cu have been shown to be effective selective catalysts for the hydrogenation of polyenes to monoenes in the hydrogenation of LO and its methyl esters. The iodine value of the partially hydrogenated linseed oil was reduced from 153 to 101 mg I_2/g.

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OP/SL04

TRANSFORMATION OF ETHANOL TO HIGHER ALCOHOLS BY TRANSITION METAL PROMOTED MG-AL MIXED OXIDES IN FLOW REACTOR

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The largest amount of fuels is produced from fossil sources especially crude oil, which are limited and their consumption is not environmentally friendly. From this reason, the scientists are looking for new ways of production fuels, especially biofuels. One of the alternatives is bioethanol, which can be used as additive to gasoline. However, the use of ethanol have two important disadvantages: (i) ethanol adsorbs water, which can cause corrosion of fuel system and (ii) has lower caloric value than gasoline. Therefore, it is not appropriate to blend ethanol with gasoline in any ratio. The problems with ethanol use as a fuel can be solved by use of higher alcohol such as butanol. Butanol is now most often produced by petrochemical process from fossil resources by hydroformylation of propylene. The coupling of ethanol by Guerbert reaction is other possibility to butanol formation. Guerbert reaction is the system of subsequence reactions: (i) dehydrogenation, (ii) aldol-condensation and (iii) hydrogenation. Each of the reaction steps need the different type of catalyst. The hydrogenation and dehydrogenation steps need the redox type of catalyst, while the aldol-condensation requires acid-based catalyst. The mixed oxides, synthesized from hydrotalcites, have good acid-based properties. The addition of transition metals such as Ni, Co, Cu, Cr, Fe, Mn, etc. causes the redox properties of mixed oxides.

The paper is focused on the use of Mg-Al mixed oxides synthesized from hydrotalcites by temperature treatment. The mixed oxides were used as heterogeneous catalyst for the conversion of ethanol to butanol in the microflow reactor. All synthesized materials were characterized by various analytics methods. The reaction was carried out at different reaction temperatures (280, 300, and 350 °C) and constant WHSV (4.5 h^{-1}). It was found that the presence of nickel, copper and cobalt positively influenced the catalyst activity. Moreover, it was found that ethanol conversion increased with increasing temperature, but in the same time decrease selectivity to butanol.

Acknowledgements
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OT/SL05

AUTOGENOUS FORMATION OF GOLD-PHOSPHORENE NANOHYBRIDS AND THEIR APPLICATION IN CATALYTIC PURIFICATION OF WASTEWATER

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Phosphorene is the single layer derivative of layered Black Phosphorus (BP), which is a member of a layered material family with anisotropic properties and with a layer-dependent bandgap. In comparison with graphene - the typical reference single layer material, phosphorene is significantly more reactive, and its reactivity can be applied for the autogenous reduction of gold ions to the metallic gold nanoparticles supported by phosphorene sheets (Au/BP). Phosphorene, as well as gold, are well-known oxidation catalysts, which are essential in organic synthesis, and catalytic treatment and purification of industrial wastewaters. The treatment of organic contaminants in water from chemical industry exhibit serious problem, and its treatment is a challenge for catalysis. Here we show a high catalytic activity of the gold-phosphorene nanohybrid (Au/BP) for wet oxidation of acrylic acid and industrial-like wastewater with complex composition. Further, the prepared nanohybrid showed high stability, which is the crucial feature for an application of layered materials, caused by a presence of gold, which modified the electronic structure of the phosphorene surface. The Au/BP stability opens the utilization of the easy-accessible surface of 2D material for the preparation of 2D material supported metal catalysts.

OT/SL06

THE EFFECT OF WATER AND SUBSTITUENTS OF AROMATIC RING ON ITS HYDROGENATION OVER A COBALT CATALYST

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The aim of this contribution lies in the experimental study of specific properties of the commercial cobalt catalyst ESM 365. The catalyst is applied in a large-capacity unit for the cyclohexylamine production in BorsodChem MCHZ, Ostrava with an existing production capacity of 18 kilotons per year. The process of production of cyclohexylamine by selective catalytic hydrogenation of aniline in gaseous phase was developed at the Department of Organic Technology of the UCT Prague. The advantages of the catalyst ESM 365 are very good utility properties: the efficient catalytic activity and selectivity and lifetime longer than a 15 years. The specific property of the catalyst is a so-called activation period. It is a period during which, under constant reaction conditions, the conversion of aniline will increase of one order of magnitude. This work presents the results of the study of activation period, characterized by parameters of initial and equilibrium conversion of aniline and time of an achieving of the equilibrium conversion. The parameter values are well reproducible and dependent on the catalyst reduction temperature and the concentration of water in the aniline. However, the reduction temperature is not related to the incompleteness of the conversion to Co^0. It has been demonstrated that the value of the parameter of the equilibrium conversion of aniline is a function of the concentration of water in aniline. The presence of water in aniline leading to significant increase of the hydrogenation reactivity of aromatic ring. Hereafter, at the identical reaction conditions the effect of substituents on the aromatic ring on the rate of its hydrogenation was studied. The reactivity for the hydrogenation of the aromatic ring decreases in the order: aniline, toluene, benzene.

OT/SL07

SYNTHESIS OF NEW RUTHENIUM COMPLEXES AND THEIR USE AS CATALYSTS IN HYDROGENATION OF DIENE COMPOUNDS

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The half-sandwich ruthenium complexes [Cp*Ru(diene compound)] $^{+}X^{-}$ are suitable and selective catalyst for the preparation of alkenes with *Z*-configuration of double bond from corresponding dienes. Ruthenium complexes **I-IX** containing acyclic, cyclic, bicyclic dienes and *α,β*-unsaturated carboxylic acids, and their derivatives as diene ligands have been successfully prepared (Fig.1). The anionic part of the complexes (X-) was represented by triflate, perchlorate and tetrafluoroborate ions.

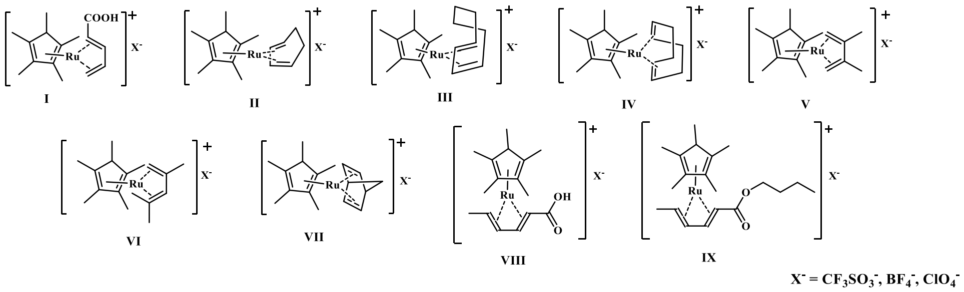

Fig. 1 Prepared Ru complexes: [Cp*Ru (2,4-pentadienoic acid)]CF_3SO_3 (**I**), [Cp*Ru (1,3-cyclohexadiene)]CF_3SO_3 (**II**), [Cp*Ru (1,3-cyclooctadiene)]CF_3SO_3 (**III**), [Cp*Ru (1,5-cyclooctadiene)]CF_3SO_3 (**IV**), [Cp*Ru (2,3-dimethyl-1,3-butadiene)]CF_3SO_3 (**V**), [Cp*Ru (2,4-dimethyl-1,3-pentadiene)]CF_3SO_3 (**VI**), [Cp*Ru (norbornadiene)]CF_3SO_3 (**VII**), [Cp*Ru (sorbic acid)]CF_3SO_3 (**VIII**) and [Cp*Ru (butyl sorbate)]CF_3SO_3 (**IX**).

Prepared complexes were used as catalysts for the selective hydrogenation of diene compounds to the corresponding products with *Z*-configuration of the double bond in a homogeneous and heterogeneous arrangement. The reaction rate was influenced by the type and the size of the diene ligand. The rate of diene hydrogenation using complexes containing isolated double bonds or bicyclic ligands was the highest. The lowest reaction rates were observed using the complexes with acyclic dienes. The influence of the type of the anionic part of the complex on the reaction rate was also studied. The lowest rate of hydrogenation was observed using the complexes with tetrafluoroborate anion. The desired products with *Z*-configuration of the double bond were formed with high selectivity (95-99 %). The results showed that the selectivity was influenced neither by the type of diene ligand nor by the type of the anionic part of the complex.

OT/SL08

PREPARATION OF α-TERPINEOL AND PERILLYL ALCOHOL USING ZEOLITE BETA

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The preparation of *α*-terpineol and perillyl alcohol by acid catalyzed hydration of limonene and acid catalyzed isomerization of *β*-pinene oxide in the presence of water was studied. *α*-Terpineol and perillyl alcohol belong to compounds with biological activity used in the pharmaceutical industry and also used as fragrances in the perfume industry. Zeolite beta (beta 25 and beta 38) was used as a catalyst. The aim of this work was to optimize the reaction conditions to achieve the highest possible conversion of reactants and the highest possible selectivity to the desired products. The studied parameters included temperature, the type and the amount of catalyst, the addition of acid, and the amount of acid in the reaction mixture. In the case of limonene hydration, we have found that the highest selectivity to *α*-terpineol was 88% with conversion 36% under the following conditions: limonene (2 ml), 50 wt% of catalyst beta 25 based on the weight of limonene, 10% aqueous acetic acid (10 ml), temperature 50°C, 24 hours. In the case of *β*-pinene oxide isomerization, it was found that the highest selectivity to perillyl alcohol, (36% at total conversion) was obtained in the reaction under the following conditions: *β*-pinene oxide (0, 8 ml), solvent dimethylsulfoxide (DMSO) volume ratio *β*-pinene oxide:DMSO 1:5, catalyst beta 25 without calcination 15 wt% calculated on the amount of *β*-pinene oxide, water molar ratio *β*-pinene oxide:H_2O 1:8, temperature 70 °C, 3 hours. The present study shows that the studied direct hydration of terpenes may be a suitable method for the selective preparation of valuable compounds from biomass based materials.

OT/SL09

SOLVENT EFFECTS IN ALDOL CONDENSATION – PRODUCTION OF IMPORTANT FRAGRANCE

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Aldol condensation is one of the methods of C-C bond formation and it is used to prepare various fine chemicals such as fragrances, insecticides, drugs, and dyes. Compounds with potential application in the perfume industry can be prepared by, e.g., aldol condensation of cinnamaldehyde with aliphatic aldehydes and subsequent hydrogenation of unsaturated aldehydes to saturated alcohols. This work aimed to find suitable conditions for the base-catalyzed aldol condensation of cinnamaldehyde with butanal followed by hydrogenation of 2-ethyl-5-phenylpenta-2,4-dienal to 2-ethyl-5-phenylpentan-1-ol. Aldol condensation was catalyzed primarily by a solution of potassium hydroxide. The hydrogenation of the obtained unsaturated aldehyde proceeded using metal catalysts mainly based on nickel.

The most interesting studied effect was the influence of the solvent. It was found that the basicity of the solvent, represented by the donor number, has a major effect on the course of aldol condensation, especially on the achieved conversion. Furthermore, a similar trend of the dependence of by-product formation on solvent basicity was observed, making methanol the most suitable solvent for aldol condensation.

The optimal conditions leading to the highest selectivity (94%) were the room temperature with the molar ratio of cinnamaldehyde to butanal 1:1 catalyzed by 10% sodium hydroxide solution (used in a molar ratio of 0.1:1 to cinnamaldehyde) and methanol as a solvent. For hydrogenation, the following conditions were selected as suitable: nickel supported catalyst (20% by weight), temperature 140 °C, and pressure 10 MPa. By optimizing this two-step reaction, a high yield of the desired product 2-ethyl-5-phenylpentan-1-ol was achieved and so this process has a potential application in the perfume industry.

ME/SL10

DIRECT LASER WRITING ON THE SURFACE OF $PbO-Bi_2O_3-Ga_2O_3$ GLASSES

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Direct laser writing can be used for modification and structuring of the materials surfaces. In glasses, this technique enables to create microlenses or craters with a potential application in optics [1]. The presence of heavy metal oxides in glasses provides suitable properties for optical applications (i.e. high linear and non-linear refractive index, high transmittance in IR region) [2].
This work deals with the role of Bi_2O_3 on microlenses and craters formation on the surface of $(PbO)_{0.75-x}(Bi_2O_3)_x(Ga_2O_3)_{0.25}$ (x = 0-0.30) bulk glasses. The prepared glasses with surface polished to the optical quality were illuminated using a focused continuous-wave laser emitting at 447 nm (diameter of beam ≈ 190 µm, maximal intensity = 430 mW). At shorter exposition times (0.1-5 s) the illuminated part of glass expanded forming microlenses. Longer exposition time (60 s) led to the formation of the craters due to the higher overheating of the illuminated area which caused the removal of the overheated material. In the case of microlenses, the low addition of Bi_2O_3 into the binary $(PbO)_{0.75}(Ga_2O_3)_{0.25}$ glassy matrix caused a significant decrease of threshold power density ($F_{th,lens}$ ≈ 1000 vs. 510 W/cm^2 for x = 0 and 0.03 within 0.1 s exposition). Subsequently $F_{th,lens}$ decreased slightly with increasing Bi_2O_3 content. Furthermore, the slope of the dependence of microlenses height on the logarithm power density (i.e. effective penetration depth) decreased with increasing exposition times for x = 0.08-0.23 and had the opposite trend comparing to that in binary $PbO-Ga_2O_3$ glasses (see [1]). The Raman and XRD measurements showed that the partial crystallization of created microlenses occurred at used longer exposition times (i.e. 0.5 and/or 5 s).
The maximal depth of prepared craters was 80 µm. The threshold power density was not significantly affected by Bi_2O_3 content ($F_{th,crater}$ = 540 W/cm^2 for x = 0 and 0.15).

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ME/SL11

PHONOLITE. AN AVAILABLE, NATURAL CZECH RESOURCE FOR PRODUCING NOVEL VALUABLE MATERIALS

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Phonolite is a volcanic rock formed mainly by alkali feldspar and other compounds. This rock is available in the Czech Republic, and it can be used as a dimension stone, aggregate for gravels, ceramics, and glass production. Because of its properties, concrete structure, and alkalinity, new uses of this resource could be found. According to the results obtained in our Research Institute, it can be used directly as an asphalt binder [1] or as catalyst support after its modification by using an acid treatment that increases its porosity and changes its structure [2, 3]. Several modified phonolite-supported catalysts containing Ni-W, Ni-Mo, and Co-Mo were tested for hydrotreatment of triglycerides and mesityl oxide. These catalysts were also tested in the hydrocracking of vacuum gas oil – vegetable oil mixtures. The experiments were carried out in an autoclave and flow reactor. Satisfactory results were found, indicating that the phonolite could be a low-cost effective valuable material for the industry especially considering that it can be obtained in a close location to the industrial area facilities in the Ústí region.

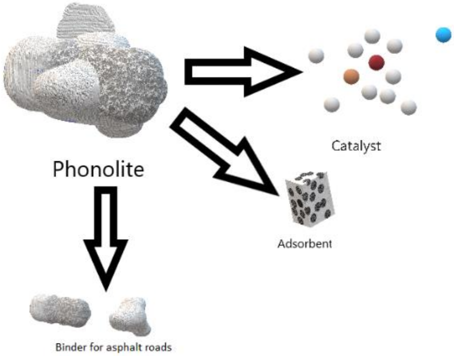

Fig. 1. Phonolite processing to new useful materials.

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ME/SL12

CHEMICAL STRUCTURE OF MoO_3-P_2O_5 BINARY GLASSES

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Phosphate glasses containing transition metals are very interesting, in addition to possible applications, also in terms of basic research. Phosphate glasses with so-called *s*- or *p*-metals are, e.g., very sensitive to moisture. This sensitivity, more precisely the hydrolysis-induced change in chemical composition towards the final orthophosphates, usually precludes their wider use. It is known that the addition of transition metals into the structure of phosphate glasses significantly improves their overall stability and thus, among other things, the mentioned resistance to moisture. Transition metals usually form a number of oxidation states and associated complex particles, which provides great flexibility in the ability to form stable glass networks reinforced by covalent coordination bonds between cations and anions, and the resulting cation-anionic structures provide high chemical and physical stability of such glasses. However, the variability of oxidation states and the formation of coordination compounds greatly complicate the study of the chemistry of such glasses, and thus the study of their structure. This then makes it difficult to select suitable chemical compositions for the possible use of these glasses. For this reason, it is necessary to focus on the behavior of transition metals in glass-forming melts of phosphate glasses.

The aim of our work was to get a basic idea of the chemistry of molybdenum and its influence in formally binary glasses MoO_3-P_2O_5 with the ratio MoO_3/P_2O_5 changing from 1/2 through 1/1, 1.33/1 to 2/1. The glasses were synthesized, elemental analysis was performed by XRF, the phosphate anionic components were characterized by ^{31}P MAS NMR, and the reduction range of Mo^{VI} to Mo^{V} was determined by EPR. From the material balance, probable chemical compounds forming glasses and their relative representation were found. The glass transition temperature, which is one of the basic characteristics of glasses in general, was also measured.

ME/SL13

CHITIN-CAFFEINE MODELS IN BIOCIDAL WOOD COATINGS

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Caffeine was confirmed as a suitable bioactive substance in the mixture against wood fungi. On the other hand, chitin is a part of fungal bodies and has been studied in previous research as a potential packing material for caffeine. For this reason, we studied caffeine interactions with chitin (in some biological tests with fungi or chitin-caffeine aquatic solutions). Caffeine concentrations in fungi and in aquatic solutions were analyzed by LC-MS and spectrometrically. SEM technique was used to visualize for image of some interactions. The results confirmed the negative effects of caffeine on fungal growth. Chemical experiment with pure chitin and caffeine indicates strong bonds of caffeine to chitin. The SEM analysis observed the ability of chitin to adhere to beech wood. The caffeine-chitin interactions were discussed from the various points of view – the effects of its protective function against pests, and application in a commercial use for the protection of wood materials.

ME/SL14

THE INFLUENCE OF LONG-TERM AGING ON STRUCTURE OF MG-AL MIXED OXIDES AND CATALYTIC ACTIVITY OF ALDOL CONDENSATION

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The Mg-Al mixed oxides are an interesting group of heterogeneous base materials prepared from hydrotalcites (anion clays). The memory effect, which causes the rebuilding of the hydrotalcite layered structure in the presence of humidity, was studied. The novelty consists in the description of influence of the long-term aging (6 months) on the structural changes of mixed oxides at ambient conditions. The structure throughout aging has been determined by several techniques, such as X-ray diffraction, DRIFT and thermogravimetric analysis. The diffraction lines of mixed oxides were observed for 91 days of aging (after that the lines of hydrotalcites started to occur). However, the specific surface area rapidly decreased after only two aging days. The change was caused by an adsorption of water and especially of carbon dioxide from the air, which formed carbonates. After 166 days, the hydrotalcite structure was fully recovered. Moreover, all aged material was applied as the heterogeneous catalyst for the aldol condensation with furfural as acid-base reaction. The conversion decreased from 72 % (immediately after the thermal treatment) to 27 % after 4 aging days. The statistical evaluation of results was also carried out and relation between variables described.

Acknowledgements:
This work was supported by the Czech Science Foundation, Project No. 19-00669S. The result was achieved using the infrastructure included in the project Efficient Use of Energy Resources Using Catalytic Processes (LM2018119) which has been financially supported by MEYS within the targeted support of large infrastructures.

ME/SL15

CONTROLLED TRIBOELECTRIFICATION OF DUST PARTICLES AS A PROMISING METHOD FOR THE IMPROVEMENT OF ELECTRODYNAMIC CLEANING SYSTEMS

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The efficiency of photovoltaic systems installed in desert or dusty areas is decreased by dust soiling. Due to the presence of adhesive forces, this accumulated dust cannot be removed by usual cleaning methods except for water-based methods; however, water is a scarce commodity in arid locations. A promising solution seems to be a device based on electrostatic repulsion, called Electrodynamic Dust Shield (EDS), which consists of a system of parallel electrodes connected to a voltage source that generates a wave, which acts as a conveyor of charged dust. Space applications have shown that EDS can achieve a cleaning efficiency of up to 90%. Despite this, compared to Mars or the Moon, the cleaning efficiency of EDS is significantly lower on Earth because different charging mechanisms apply on our planet. Researchers believe that it is important to increase the Coulomb force in the system. That is why studies of EDS optimization are focused especially on the system configuration, i.e., the distribution and magnitude of the electric field. However, the static charge carried by dust particles is of the same importance in Coulomb force, and the control of charge magnitude and polarity could help to increase the cleaning efficiency even in cases when the further increase of field strength is not possible, e.g., because of the breakdown of air. Static charge on particles is generated mainly in three steps:

(I) by ions in the presence of the electric field,
(II) due to tribocharging during mutual collisions of airborne sand particles,
(III) due to tribocharging of particles and the EDS surface.

Steps (I) and (II) are highly difficult to control in the real system, however, we believe that step (III) can be modified by changing the properties of the charging counter material, i.e., the surface of EDS. In this study, we present a methodology enabling us to evaluate the significance of tribocharging for fine powders. We confirmed that the bipolar charge obtained during step (II) cannot be sufficiently controlled in step (III) by a commonly used EDS surface; however, with the utilisation of thin films prepared by electrospraying, we are able to control both the polarity and the magnitude of the charge on dust particles.

SP/SL16

RHEOLOGICAL PROPERTIES OF POWDER MIXTURES AS A FACTOR OF HARD-GELATIN CAPSULE FILLING PERFORMANCE

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Hard gelatin capsules are commonly used dosage form. For larger-scale productions, there are several types of automated capsule filling equipment. The two most used types of filling machines operate using dosing disc and dosator concepts. Each type works in different operation regime and under different conditions. Therefore, the requirements on the powder flow properties can be quite complex and need to be studied and adapted to the specific filling technique for failsafe operations.

Given the knowledge of complexity of flow property requirement, the objective of this study is to deliver a case study dealing with investigation and optimization of real powder mixture for capsule filling in different types of machines. The mixture composes of active pharmaceutical ingredient (API), corn starch and liquid dimethicone. It is prepared in several steps including creation of premix (dimethicone and a defined amount of starch), active mixture (API and dimethicone) and their mixing with remaining starch to obtain final mixture. In addition to the original mixture, several modified mixtures were evaluated differing in the mixing time of final mixture and the amount of starch in premix. Rheological properties were characterized using powder rheometer FT4 data and Carr's compressibility index (CI). Main attention was paid to influence of premix preparation and final mixture mixing time. Obtained values of CI occurred in range 30-48 %. Lower values corresponded to mixtures with shorter mixing time and higher amount of starch in premix indicating their better flow properties. Based on the fundamental literature suggesting optimal value of CI in range 18-30 % (dosing disc) and in range 25-35 % (dosator), the best flowing mixtures were supposed to be successfully processable using dosator. In case of dosing disc, no mixture met the criteria required. Further optimization or re-formulation is necessary to process the formulation in this type of filling machines.

SP/SL17

TABLET MICROSTRUCTURE EVOLUTION DURING THE COMPACTION PROCESS

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Direct compaction of bulk powder mixtures is a complex process with a significant influence on the final tablet structure and subsequently also its performance during disintegration and drug release. More specifically, particle rearrangement, deformation or fragmentation take place during the compaction. However, these effects do not necessarily depend only on individual materials properties, the final product composition and the compaction process parameters are also crucial. Understanding and description of the final product properties and their dependency on individual material selection and compaction settings can therefore be very useful in the drug formulation or compaction process development and this study was aimed at improvement of one aspect of this understanding.

Viscoelasticity is one of the most significant material properties having the ability to influence final tablet properties. Therefore, materials for model mixtures were chosen based on Young modules during compaction in the presented work. The combination of a hard, brittle excipient and a plastically deformable drug was in the centre of attention. The choice was made based on the premise of the brittle material being protected from fragmentation by the plastic one, when present in a sufficient amount. This work aimed to present a methodology to describe such phenomena, which can be further used in practical applications.

Series of tablets were prepared from the model materials having different compositions and used compaction loads. They have been further analyzed with a scanning electron microscopy (SEM) for cross-section areas microstructure and with a flow-through dissolution for disintegration and dissolution properties.

Presented model binary mixtures proved the premise about the protective function of plastic material, when present as a major mixture component. However, further work is planned to complete the methodology with different material combinations and to ultimately use it for practical tablet formulation development.

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SP/SL18

APPLICATION OF HANSEN SOLUBILITY PARAMETERS IN PHARMACEUTICAL INDUSTRY

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In the pharmaceutical industry, the solubility of API in water is very crucial. Poor water solubility often leads to poor bioavailability. To provide safe, quality and effective drugs to patients, the bioavailability of API must be enhanced by a suitable drug formulation.

Preformulation chemists often count on their empiric experiences with certain excipients, which may enhance the API solubility. Usually, the chosen formulation is not suitable for API in terms of API recrystallization to the other crystal systems (and hereby the patent collision) or the inappropriate interaction between API and some excipients. This problem can be prevented by using Hansen solubility parameters, making the preformulation process more effective and simultaneously speeding up the launch of the drug products on the market. Hansen solubility parameters (HSPs) could be the future of preformulation development when its "likeness" can determine the suitability or rather compatibility between API and excipients. The HSPs of measured excipients will create a "library". According to the Hansen theory, the HSPs of API will be determined, and the compatible excipients to API will be assigned.

This work aimed to verify predictions of compatibility between selected APIs and chosen polymers to enhance the APIs' bioavailability. The first step was to determine the HSPs of selected APIs which were poorly soluble in water. In this work, solubility parameters of excipients were measured using the solvent method, and solubility parameters of APIs were determined by inverse gas chromatography (IGC). The compatible polymers for measured APIs were chosen according to their distance in Hansen 3D space, which is represented by the *Ra* parameter. The goal was to formulate APIs with compatible polymers into amorphous solid solutions using hot-melt extrusion. Subsequently, the amorphous solid solutions were subjected to dissolution tests to investigate the bioavailability of selected APIs. The dissolution tests confirmed that the APIs' bioavailability was enhanced, showing the effectiveness of the prediction model based on the Hansen theory.

SP/SL19

CERAMIDE LIPOSOMES: FORMULATION OF STRATUM CORNEUM LIPIDS FOR SKIN BARRIER RECOVERY

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Atopic dermatitis and psoriasis are skin diseases caused by lowered levels of skin lipids, namely ceramides, in the stratum corneum lipid matrix. Viable alternative to the conventional corticosteroids is topical delivery of appropriately formulated skin lipids. For this purpose, we developed unique ceramide liposomes (cerosomes) with excellent efficiency in disrupted skin barrier repair. Thin lipid film hydration and high pressure homogenization were used to prepare various types of liposomal systems. To determine the stability, the particle size and polydispersity index were measured. The optimal systems were found to include ceramide 3 and 6, cholesterol and stearic acid, with 10% urea in phosphate-buffered saline as the aqueous phase. Next, the ability of the system to repair chemically-damaged porcine skin was tested. While treatment by a standard lipid suspension reduced the passage of a model permeant only to a limited extent, drug flux through the liposomally-treated skin was much closer to permeation through intact skin. The non-homogenized liposomes were more effective than their homogenized version. These findings were also confirmed by FTIR measurements. This suggests that our approach to liposomal development has considerable potential for the repair of a disrupted skin barrier.

The work was supported by the Czech Science Foundation (GACR19-09600S).

SP/SL20

MORPHOLINE DERIVATIVES: NOVEL SUBSTANCES FOR MODULATING THE PERMEABILITY OF THE SKIN BARRIER

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Transdermal drug delivery is an attractive non-invasive method offering numerous advantages to conventional routes of administration, mainly due to elimination of side effects. However, the main obstacle for drugs entering the skin is its uppermost layer, the *stratum corneum* (SC). To facilitate drug transport through this barrier, the passage can be modulated by transdermal penetration enhancers that are able to influence the skin barrier resistance. In this study, we investigated the enhancing activity of a series of morpholine derivatives. We tested these compounds with three model drugs differing in their physicochemical properties. Theophylline represented small molecules with balanced hydrophilicity; indomethacin and diclofenac were selected as larger lipophilic representatives differing in their solubility. All the examined enhancers were efficient; however, it was evaluated that the most effective enhancers were the ones with 10, 12 and 14 carbons in their side chain. The results also showed a bell-like relationship between the enhancing activity and the hydrocarbon chain length of the morpholine derivatives. To further asses the properties of our enhancers, we tested their influence on permeants´ solubility and on the barrier function of enhancer-treated skin. Moreover, cellular toxicity on spontaneously immortalized human keratinocytes (HaCaT) cell line was determined and the interaction of derivatives with skin at the molecular level was examined by FTIR spectroscopy for the most effective enhancers. Therefore, in this study we submit a comprehensive summary of the properties of morpholine derivatives identifying them as candidates for effective transdermal application.

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SP/SL21

IMPROVING DISSOLUTION RATE OF POORLY SOLUBLE DRUGS BY MILLING AND CO-MILLING TECHNIQUE

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Milling of APIs alone or co-milling of APIs with an excipient are used as one of the efficient techniques that improve physicochemical properties such as solubility and dissolution rate. The enhancement of the solubility may be caused by the drug amorphization. Each drug has a different ability to form an amorphous phase (glass forming ability). And the influence of excipients is also crucial because the proper choice thereof increases the dissolution rates of API.

The aim of this work was to compare the behavior of drugs having different glass forming ability. Mefenamic acid was chosen as a non-glass forming model drug and indomethacin as a model glass forming drug. Firstly, APIs were milled alone and then mixed with one of the appropriate excipient (Ac-Di-Sol, meglumine, or PVP). Secondly, the APIs were co-milled as binary mixtures with the same excipients. Finally, both techniques were compared in terms of dissolution and surface properties.

Our results indicate that co-milling is a valuable approach in enhancing the dissolution rates of poorly water-soluble APIs. Co-milling results in a much faster release of the API than its milling itself and subsequent mixing with the excipient. Also, the effect of excipient type on dissolution rate was observed. Finally, it was found that the glass forming ability of drugs significantly affects their surface properties.

SP/SL22

POSSIBILIES AND LIMITATIONS OF ELECTROANALYTICAL METHODS IN PHARMACEUTICAL ANALYSIS

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The presentation will be focused on so far untapped potential of modern voltammetric and amperometric methods in pharmaceutical analysis and on the possibilities how to circumvent problems preventing wider use of electroanalytical methods in this field. Attention will be paid to the search for:

i) new electrode materials, their structural characterization, pretreatment and practical application in pharmaceutical analysis,
ii) new methods eliminating passivation of electrode surface, which is the biggest problem in practical application of modern voltammetric and/or amperometric methods,
iii) new electroanalytical methods in flowing systems increasing the productivity of analytical measurements,
iv) new methods suitable for monitoring of drugs and their metabolites in biological and environmental matrices,
v) new ways of interaction of industry and academia in research and development

At the end, an attempt for prediction regarding further development of the use of electroanalytical methods in pharmaceutical analysis will be made.

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SP/SL23

BATCH OR CONTINUOUS CRYSTALLIZATION & THEIR EFFECT ON PHYSICOCHEMICAL PPROPERTIES OF SOLID PHASE

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In pharmaceutical industry, crystallization is final step of producing active pharmaceutical ingredients (APIs) and is used as both separation and purification process. Traditionally, crystallization of APIs has been undertaken in batches. Batch processes can demonstrate significant batch-to-batch variability in product quality. Therefore, there is interest in moving these processes into a continuous operation. Continuous crystallization offers advantages such as greater control of particle size distribution (PSD), easier scale-up and reduction in operating costs.

Nowadays, wide ranges of crystallization methods are known (cooling crystallization, antisolvent addition or sonocrystallization). The type of crystallization influences physicochemical properties of final solid form. During batch crystallization, we are able to control PSD and amount of residual solvents by seeding; we can affect surface properties by sonocrystallization. Production of dry powder inhalers must have PSD in a range of micrometres. In all cases of batch crystallizations, micronization is required to reduce PSD. We are not able to prepare such small crystals. Some crystallization methods are preferable to prepare solid with a high Young’s modulus. The higher the Young’s modulus the easier micronization and fewer steps are needed. However, it is not possible to avoid micronization process after batch crystallization. On the other hand, continuous crystallization represents one possible way to avoid micronization. Crystal’s surfaces are affected during micronization, the more micronization cycles the greater material loss and the more expensive production is.

Fluticasone propionate was chosen as a model substance which is crystallized by adding water as antisolvent. Continuous crystallization was performed in different arrangements. Water-fluticasone propionate solution ratio and reaction cell were changed, ultrasound was used in pulsation or continuous mode and amplitude of ultrasound was changed. As result, crystals in micrometre size were obtained. After optimization of the process, micronization will not be required in continuous crystallization.

EC/SL24

SOUČASNÉ TRENDY CHEMICKÉHO PRŮMYSLU V ČR

Souček I.

SCHP ČR

V rámci komentářů k současným trendům chemického průmyslu ČR se práce zaměřuje na následujícící témata:

- Stav chemického průmyslu ČR – 2020
- Vývoj chemického průmyslu EU v posledních letech
- Potenciální směry vývoje chemického průmyslu
- Spolupráce s MPO: Studie dekarbonizace, Vodíková strategie
- Dopady pandemie

Kontext komentářů k rozpracované studii dekarbonizace a vodíkové strategii ČR vyplývá z nutné transpozice evropské legislativy zarámované „Zelenou dohodou“ – Green Dealem (EGD).

EC/SL25

TECHNO-ECONOMIC OPTIMIZATION OF STEAM CRACKER'S STEAM NETWORK

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Challenging market environment, tightening customers' requirements as well as commitment to reduce the environmental impact make the energy efficiency a very actual topic. In the petrochemical industry, energy costs are the second largest expenditure right after the feedstock. Examined Steam Cracker´s (SC) steam network in SLOVNAFT refinery operates on six steam pressure levels and includes auxiliary steam boiler, steam-cracking furnaces with steam generators, a dozen of back-pressure or combined condensing/extraction steam turbines and steam let-downs. This steam network is quite flexible, which allows operating as a standalone network or import, alternatively export, steam from/to outer network. Outer steam network is fed by steam from Combined Heat and Power Unit (CHP) as well as from secondary steam sources located in the refinery. This layout complexity and operation flexibility offers the possibility for overall techno-economic optimization reflecting both technical limitations and actual economic situation. This study provides a brief comparison of its operation before and after debottlenecking (implementation of regulation valve) and shows the importance of proper regulation possibility. Proposed calculation methodology of savings resulting from debottlenecking confirmed an advantageous economy, with the annual savings reaching up to 1 million € and the simple payback period being less than 1 year. Propriate key performance indicators (KPI) were also determined to assess the overall steam network performance as to maximize energy efficiency and savings.

EC/SL26

DIGITAL WELL-BEING FOR HIGHLY SKILLED STAFF

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Research background: Growing scientific evidence from workers in digital environments has shown that devices' unconstrained use can have substantial negative consequences. Multitasking and constant notifications are associated with lower levels of creativity and concentration; the difficulty of effective interpersonal communication causes higher stress, while heavy screen use is linked to eyesight problems and headaches. These issues are caused both by the technology and organizational expectations, leading to deterioration in productivity/performance and employees' mental and physical health.
The COVID19 and the Czech government administration measures have fundamentally affected daily pedagogical life and research at higher education institutions (HEIs). Public expectations generate moral pressure on university management to ensure a smooth pedagogical process. The University of Chemistry and Technology, Prague, mastered the transition to distance learning using the e-learning system and the MS Teams; however, without addressing lecturers' working conditions in the home office. The risks for the quality of education mean dealing with lecturers' digital well-being who will support e-learning platforms on an open university's principle or teach in a work regime 24/7.
Purpose of the article: Many large corporations are already addressing digital overload via well-being policies within their human resource/corporate social responsibility work. Some high-profile higher education institutions have also developed policies. However, research showed that no HEI providers had developed structured support for teaching staff on the topic.
Methods: The methodology insists on several ways that enable a triangular analysis. The research combines in-depth-analysis of bibliographic data in the Web of Science and Scopus databases, narrative cases based on semi-structured interviews with top managers/co-owners of companies and higher education lecturers.
Findings & Value added: The digital economy will transform the labor market and bring new forms of labor relations between employers and employees, impacting health and safety protection or the reconciliation of work-life balance. Distance teaching will be a substantial part of the pedagogic job due to pandemic measures, and secondly, Education 4.0. Czech, public universities resolved the responsibility for safe performance management by a contractual arrangement between the employer and the employees. The agreements respect the labor law provisions dealing with health and safety at work in the case of a home office. The findings focus on the risks of distance work at HEIs, i.e., physical, mental, social risks, and HR practices applicable to their prevention.
Keywords: Higher education institution, lecturers, digital well-being, risk prevention
JEL Classification: I23; I31; M14

EC/SL27

PERSONAL AND TRANSVERSAL COMPETENCIES IN BIO-BASED ECONOMY

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Decarbonization, the use of alternative raw materials including waste, biofuels and other non-food bioproducts, the use of biochemical processes - these are all current trends to which technology development and research, as well as company management, must respond. However, this is not just a financial issue but a competence one as well, since it is important to help employees acquire the necessary competencies to successfully implement these current trends within the modern workplace.

As part of the BioComp project, an analysis of competencies experts consider to be the most important for workers in the bio-based economy was carried out. Interviews were conducted with experts in bio-based fields in the spring of 2020. 139 respondents from eight European Union countries took part. Competences were monitored in three areas, namely Personal, Transversal, and Technical.

The research was conducted via questionnaire, the respondents had the task of assigning a score of one to ten points to determine the importance of individual competencies within bio-based industries. The questionnaire was created based on previous interviews conducted with experts from the bio-based economy.

The results show that the chosen competencies are considered very important by the addressed experts. The average rating in the category of Personal competencies was 8.41 and in the category of Transversal competencies 8.31, with 10 being an extremely important competence.

The BioComp project is currently developing learning scenarios to support the acquisition of the most important recorded competencies.

EC/SL28

CONSUMER ATTITUDES TOWARDS HOUSEHOLD WASTE SORTING

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Manufacturers of consumer chemicals have been endeavouring in recent years to increase the sustainability of their product packaging. They apply various strategies, in particular reduce, reuse and recycle. The recycle strategy is focused primarily on the introduction of packaging from reusable materials and the use of recycled material in the production of packaging. Both of these options presuppose the cooperation of final consumers. Their willingness to assist recycling, especially in the sorting phase, affects both the quality and quantity of recycled material and the efficiency of the recycling process. The role of final consumers in relation to the recycling process and household waste sorting has not yet been addressed in the literature. Therefore, a primary quantitative research was conducted among 350 users of consumer chemicals aimed at finding out their attitudes to individual activities in the sorting of household waste. The individual activities were compared according to the willingness of consumers to perform them, identifying activities that consumers are most willing to do. The results of this research not only enrich the theoretical level of knowledge in the field of environmental behaviour of consumers, but also help to set up reverse logistics systems.

EC/SL29

SYSTEM MODEL OF MAITENANCE DYNAMICS

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Facility maintenance became one of the most important factor which influences the profitability of companies with continuous production processes. Therefore, the facility management is the important task for the production department. The paper describes the sources of dynamics in this complex problem. The tool for the description is causal loop approach that identifies the back-loops. These loops include the planned maintenance and solving ad-hoc problems, it means repairs of defects in the production line. The system has the features of operation management and project management. For both issues it is necessary to solve the problem of resources and costs. The dynamic model is built as a system dynamics model where the main parameters are calculated. The key flows are the defect creation and also the defect elimination by means of planned maintenance and through repairs. The presented graphs demonstrate the changes of main parameters included in the model. The model can help to find the strategy for both kind of maintenance and can be used as education aid for understanding the dynamic of the described topic.

AP/SL30

INNOVATIVE TECHNOLOGY PLASMICAT FOR HAZARDOUS AIR TREATMENT

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The environment or directly human health can be threatened by air pollutants not only due to regular air industrial emissions, but also from sudden massive chemical release due to inappropriate handling. Besides fundamental prevention measures, air could be treated to minimize the damaging consequences of such events. Current air decontamination technologies don't meet all required features such as reliability, stability or autonomy in addition to efficiency, versatility and deployment speed. For safety or environmental engineering applications, we developed an innovative technology based on microwave generated atmospheric plasma combined with microwave assisted catalytic oxidation. Microwave irradiation in chemistry enables many specific effects which can result in some process improvements, especially in heterogeneous catalysis. Moreover, a new mixed cobalt-manganese oxide catalyst was applied as a lower cost available material with a high activity. Using a new build dedicated pilot demonstration unit, the technology performance and parameters were tested and verified at simulated conditions close to its real industrial implementation. This contribution introduces this unique PLASMICAT technology and presents results from two series of model simulations.

In the first experiments, we tested the efficiency of technology in the destruction of several VOCs representing various chemical structures under different temperatures and air flow rates. The achieved data confirmed the versatility of the process, being efficient even for persistent tetrachloroethylene contamination, while the destruction of different chemical bonds is controlled especially by catalyst temperature and airflow. The applied pilot 12 kW unit is designed to clean up the air stream up to 2.5 m^3/min and 300 °C. Then, PLASMICAT was implemented in the decontamination simulation of indoor chemical release of phosgene and sarin simulant at NINCBP Institute. The results of these experiments with 500 ppm contamination of 60 m^3 verified the high potential of the technology for rapid elimination of such big threat.

BI/SL31

MEAT FROM PETRI DISH

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Recently, the so-called cultivated meat (meat from a petri dish), i.e animal cells cultured in vitro in a synthetic medium, has aroused interest. This option is tempting for many reasons, but so far it is a technology that is in the research stage rather than a real alternative to ordinary meat. However, the first swallow is chicken grown in this way, which has been approved for sale to regular customers in Singapore.

The lecture will present the current state of the field from the selection of a suitable type of animal cells, through the composition of the culture medium to special types of bioreactors / culture systems. Attention will also be paid to the problem of how to force animal cells to grow in multiple layers and thus create a structure similar to a regular steak. Ethical, nutritional, legislative and other issues related to this completely new field will also be discussed.

BI/SL32

BIOSYNTHESIS OF METAL NANOPARTICLES USING *VITIS VINIFERA* EXTRACT AND THEIR ANTIMICROBIAL ACTIVITY

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Nowadays, medicine faces challenges related to the spread of antibiotic resistance. One of the possible solutions to this problem could be the use of metal nanoparticles, objects with dimensions below 100 nm. Due to the high surface to volume ratio, nanoparticles have exceptional properties, including antimicrobial activity. In general, metal nanoparticles can be prepared in three ways: chemically, physically, and biologically. The biological route is the most eco-friendly and cost-effective of the mentioned methods. This study aims to biosynthesize gold nanoparticles using *Vitis vinifera* extract and to determinate their antimicrobial activity. The extract was prepared using viticultural waste, specifically the dried canes of *V. vinifera*. The obtained nanoparticles were characterized using UV-VIS spectroscopy and transmission electron microscopy (TEM). TEM analysis showed that the nanoparticles had heterogenous shape and size mostly in the range from 8 to 22 nm. Subsequently, the effect of nanoparticles on planktonic cells of two strains of *Pseudomonas aeruginosa* was studied. The antimicrobial activity of the nanoparticles varied depending on the tested strain of the microorganism.

BI/SL33

GENUS *MONASCUS* AND ITS SECONDARY METABOLITES

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Genus *Monascus* belongs to the kingdom Fungi. These ascomycetes are known and used in Asia for centuries. They are used for food dyeing and conservation or as a part of traditional Chinese medicine. In the western world, *Monascus* fungus is nowadays used to produce food supplements that prevent hypercholesterolemia and cardiovascular diseases. The representatives of the genus *Monascus* produce a wide range of primary and secondary metabolites, some of them having significant biological effects. The most important metabolites are pigments, monacolins, and mycotoxin citrnin. Other metabolites are, for example, γ-aminobutyric acid, dimerumic acid, or ethanol. *Monascus* pigments are polyketides with antiproliferative, anti-inflammatory, or antimicrobial effects. Monacolins belong to the group of statins, they inhibit the activity of 3-hydroxy-3-methylglutaryl-coenzyme A reductase. HMG-CoA reductase plays a significant role in cholesterol biosynthesis. Mycotoxin citrinin has nephrotoxic and hepatotoxic effects. The use of the genus *Monascus* mainly in the food industry has a large potential, however, the problem with the production of undesirable compounds such as citrinin has to be solved.

BI/SL34

ANTIMICROBIAL AND ANTIVIRULENCE ACTIVITY OF PTEROSTILBENE, METHOXYLATED DERIVATIVE OF RESVERATROL

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Antibiotic resistance among microorganisms represents an urgent problem of today clinical practice. With common antibiotics failing to cure infectious diseases caused by resistant pathogens, an alternative strategy for their treatment emerged acting via inhibition of infectious properties of the pathogens rather than their killing. Virulence enables pathogen to cause host infection in the first place, to further promote it and colonize other host tissues and effectively evade host immune system. The virulence factors comprise of various toxins, extracellular enzymes or adhesins. Biofilm formation and morphology switching act also as a manifestation of virulence in pathogen. Therapeutics capable of suppression of virulence could enhance modern antibiotic therapy and effectively treat infections caused by these otherwise persistent untreatable microbes.

Pterostilbene, a natural antioxidant found in various plants (*Vaccinium* berries, bark of *Pterocarpus* trees or in wine grapes) has a wide spectrum of beneficial pharmacological effects, among which the most outstanding is the antimicrobial combinatory activity with antibiotics. In this study, its effect was observed on *Staphylococcus aureus* and *Staphylocccus epidermidis* as well as *Candida albicans*, which stand as important examples of both resistant pathogenic bacteria and yeast. The effect of pterostilbene alone and in combination with erythromycin was studied on suspension growth and biofilm formation of mentioned species. Its antivirulence effect on production of extracellular virulence factors (proteases, phospholipases, haemolysins etc.) was further examined by agar plate and colorimetric methods. The results were supported by scanning electron or fluorescent microscopy.

Pterostilbene was found to have permeabilization activity on cell membranes in *Staphylococcus* spp., which is likely crucial for potent synergistic activity with antibiotics. The biofilm formation was supressed as proved also by fluorescent microscopy and decreased haemolytic activity of *S. epidermidis*. Pterostilbene was proved to have antivirulence activity on genus *Staphylococcus* and the enhancement of antibiotics activity was shown to be very beneficial.

BI/SL35

EFFECTS OF *VITIS VINIFERA* EXTRACTS ON REPRESENTATIVES OF GASTROINTESTINAL TRACT-ASSOCIATED MICROORGANISMS

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The waste products of the wine industry are neglected materials with the potential for wide pharmaceutical use. By-product of *Vitis vinifera* cultivation, i.e. the canes, are an important source of bioactive substances - polyphenols. In recent years, polyphenol compounds are a subject of increasing scientific interest, mainly due to their variety of potential beneficial effects on human health, such as the influence on the composition of human microbiome. This study was aimed at the effect of polyphenols contained in extracts of *Vitis vinifera* canes, on selected probiotic and opportunistic pathogenic bacteria closely related to the human digestive tract. The cane extract was prepared, characterized and the effect on the change in biofilm formation of opportunistic pathogens (e.g. *Escherichia coli*, *Citrobacter freundii*) and probiotic bacteria (e.g. *Lactobacillus acidophilus*) was observed. The minimum inhibitory concentrations (MIC_{50} and MIC_{80}) were determined for the planktonic populations of microorganisms. The metabolic activity of biofilm cells was evaluated by the MTT viability assay. The effect of vine grape cane extract varied when applied on probiotic and opportunistic pathogenic planktonic and biofilm cells of studied strains. The *Vitis vinifera* cane extract induced the planktonic growth in probiotic strain *L. acidophilus* while successfully inhibiting the growth of both opportunistic pathogenic microorganisms (*C. freundii* and *E. coli*). Polyphenol supplementation by the extract from canes stimulated the biofilm formation of the beneficent genus *Lactobacillus,* but inhibited both of the opportunistic pathogenic species. By applying *Vitis vinifera* cane extract at a concentration of 500 mg_{GA}/L of total polyphenols, the metabolic activity of biofilm cells of both opportunistic pathogens was reduced by at least 80 %, while the probiotic strain was not negatively affected by this concentration.

BI/SL36

ANTIMICROBIAL ACTIVITY OF CHITOSAN NANOPARTICLES AGAINST *PSEUDOMONAS AERUGINOSA*

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Due to the growing prevalence of highly resistant bacterial strains, there is an increasing need for new treatment approaches that would at least reduce the pressure on the development and use of antibiotics. Very promising is the quorum quenching strategy, which aims primarily to suppress pathogenicity without causing bacteriostatic or bactericidal effects. The principle consists in modulating the communication mechanism of quorum sensing, in which signalling compounds called autoinducers are produced and released in response to fluctuations in cell population density. A representative of the quorum sensing bacterium is the gram-negative pathogen *Pseudomonas aeruginosa* communicating via acyl-homoserine lactones. After reaching a minimal threshold stimulatory concentration, these simple membrane diffusion molecules affect gene expression and phenotype, which are key to the ability of the bacterium to cause serious chronic infections. By finding quorum quenching agents, we could obtain a powerful tool in the treatment of pseudomonal infection. One of the substances interfering with the quorum sensing system of *Pseudomonas aeruginosa* and antibiofilm activity is chitosan. Structurally, it is a copolymer of D-glucosamine and *N*-acetyl-D-glucosamine units obtained by deacetylation of chitin. Since the effect of chitosan is strongly conditioned by molecular weight, the degree of deacetylation, and finally, the type of microorganism tested, it offers the opportunity to study the chitosan effect in the form of nanoparticles. Compare to chitosan, its nanoparticles have a higher surface charge density, which enhances the antimicrobial effect. In addition, the nanoscale provides the benefit of improving biocompatibility and can prevent unwanted interactions with the immune system. Due to the nontoxic nature and good biodegradability of chitosan, its nanoparticles have a wide potential for use as a carrier for various therapeutics, including proteins, vaccines, or DNA.

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BI/SL37

PRODUKCIA ENZÝMOV LIPOXYGENÁZOVEJ DRÁHY POMOCOU REKOMBINANTNEJ *E. COLI*

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Súčasné zameranie technológií na udržateľné procesy prinieslo do popredia použitie multienzymatických kaskádových procesov, pri ktorých nie je nutné separovať medziprodukty. Každá priemyselná aplikácia má svoje špecifické požiadavky na parametre bikatalyzátora – jeho čistotu, aktivitu, formu aplikácie. Dôležitým parametrom biokatalýzy je samotná cena enzýmu, ktorá závisí najmä od spôsobu jeho prípravy, potreby izolácie a možnosti viacnásobného použitia.

Lipoxygenázová dráha je zdrojom C6 a C9 aldehydov slúžiacich ako senzorické molekuly. Jej produkty patria do oxolipínového metabolizmu, ktorý je zapojený do obranných mechanizmov rastlín.

Poznatky o príprave a charakterizácii lipoxygenázy sú dobre dostupné, no napriek tomu sa pri syntézach hydroperoxidov pre hydroperoxid lyázu (HPL) stále používa ako jej zdroj sójová múka. Ako problematická sa však ukazuje produkcia samotnej HPL. Keďže patrí do skupiny cytochrómov P450, potrebuje pre svoju katalytickú aktivitu hém ako prostetickú skupinu.

Rýchla produkcia rekombinantného proteínu počas jeho expresie predbieha biosyntetickú dráhu hému v *Escherichia coli* a tvorí sa neaktívny proteín. Predpokladá sa, že limitujúcim krokom v metabolizme hému je vznik kyseliny δ-aminolevulovej.

Táto práca bola podporená Agentúrou na podporu výskumu a vývoja na základe Zmluvy č. APVV-18-0254. Táto publikácia vznikla vďaka podpore v rámci Operačného programu Integrovaná infraštruktúra pre projekt: „Strategický výskum v oblasti SMART monitoringu, liečby a preventívnej ochrany pred koronavírusom (SARS-CoV-2)", Kód ITMS2014+: NFP313011ASS8, spolufinancovaný zo zdrojov Európskeho fondu regionálneho rozvoja.“ ,

PC/SL38

DEACIDIFICATION AND PRESERVATION OF CELLULOSIC OBJECTS OF CULTURAL HERITAGE

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The industrial progress in papermaking in the early 19th century led to technologies using alum ($KAl(SO_4)_2$) and rosin (abietic acid being the main component of it) [1]. Consequently, papers became acidic and degradation processes have proceeded more rapidly. Splitting of cellulosic chains by hydrolysis and oxidation - including microbiological effects, are the main processes resulting in a decrease of mechanical strength and the changes of colour[2]. The application of sizing agents amplified hydrophobic/hydrophilic differences between the properties of the surface and the bulk of the paper as well. These facts necessitate an application of either polar (water-based) or non-polar (alkanes, perfluoralkanes, hexametyldisiloxane and similar) deacidification systems. In the first stage, the deacidification components themselves (magnesium and calcium species, amines, etc.) come to the surface. Polar systems allow to swell cellulosic bundles and soluble deacidification components (e.g. $Mg(HCO_3)_2$) can diffuse to interior of paper sheets. In case of non-polar systems, e.g., $Mg(OCH_2CH_3)_2$ in an organic solvent, a hydrophobic step is applied firstly, and after penetration of potentially deacidification species to the volume of a paper sheet, “hydrophilic steps” takes place under action of water vapours. When properly performed this procedure, a uniform distribution of deacidification agents in the body of paper may be obtained[3,4]. As a continuation of the project KnihaSk[5], we got involved in the solution of the outlined problems in the framework of the project: “Synthesis, compatibilization and transport of components of multifunctional systems suitable for the stabilization of cellulosic materials”. Focus is on mass transport phenomena, chemical transformation of potentially deacidification species and a final effectiveness of the used systems.

Acknowledgement:

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PC/SL39

IT´S ALL MADE OF PLASTIC – THE EFFICIENCY BOOST FOR POLYMER INDUSTRY WITH VIBRATION SPECTROSCOPY

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«Plastic» has become somewhat of a dirty word. It makes us think of trash and environmental pollution, inferior quality, mass-produced goods, and excess. For example chemical manufacturing such as polyurethane production is characterized by a cost intensive production process combined with severe adverse ecological effects.
But if you take a look around, you will realize that a lot of the objects that surround us – including those that we couldn't live without – are also made of plastic. That's no accident: as synthetic organic polymers, plastics have the advantage that their properties can be perfectly adapted to their intended use – unlike most natural materials – and they can also be manufactured inexpensively. Thanks to their versatility, plastics have become established in all areas of our lives. Whatever their use – whether it is food packaging, flooring, or textile fibers – plastics have to meet quality criteria which are often determined by standards. To ensure that they satisfy the quality requirements, analysis must be carried out at every stage of production, from the raw materials in the warehouse to the reaction conditions and intermediate products in the process, right up to the final products.

All these quality control steps can be significantly improved by using vibrational spectroscopy such as near infrared spectroscopy and Raman Spectroscopy. These analytical techniques can assist the operator of the plant to reduce costs and minimize the impact on the environment, which should be one of our world priorities nowadays.
Near infrared spectroscopy and Raman spectroscopy are an easy and fast analysis techniques, which can replace the time-consuming conventional lab methods down to minutes instead of hours and help to keep the process flow in good conditions required by audit departments. Such as in the 2012 guidance from the European Medicines Agency on Real-Time Release testing is described the ability to control processes to make consistent product through data verification during production and process understanding and control is recognized

Aims of this research were to reduce the environmental demand of production of polymers, the rise of the efficiency of quality control, optimizing conditions for production stream as well as reduction of production costs by the use of vibration spectroscopy in the polymer industry.

PC/SL40

PREPARATION OF MICRO-CELLULAR BIOPOLYMERIC FOAMS BY THERMALLY INDUCED PHASE SEPARATION (TIPS)

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Polymeric foams are widely used materials due to their various application possibilities. Based on their morphology, they can be used as thermal or sound insulators or as memory foams in bed mattresses. With decreasing pore size, thermal and sound insulation properties improve, and moreover other application possibilities become viable, e.g., membranes, scaffolds in tissue engineering or solid support in biosynthesis. This contribution deals with preparation of micro-cellular foams from biodegradable poly(lactic acid) (PLA) by unconventional method of thermally induced phase separation.

TIPS is a flexible method allowing preparation of porous materials with open-pore structure, closed-pore structure or even their combination. It consists of three basic steps: 1) dissolution of the polymer in the solvent, 2) temperature quench of the solution well below its freezing point leading to limited phase separation and solidification, 3) frozen solvent removal. After the solvent removal, a porous polymer matrix is obtained with morphology greatly influenced by chosen process conditions (e.g., rate of cooling, initial composition of the polymer-solvent solution). Therefore, this method allows good control of the final morphology, which is essential in scaffold engineering, as the ideal scaffold morphology changes with the tissue type.

PLA was dissolved in acetic acid (AA) which was – to the best of our knowledge – used as a TIPS solvent for the first time. Foaming was done at five different concentrations of PLA in AA (8%, 10%, 12%, 14% and 16% wt.) and the frozen AA was removed by extraction, while various extraction agents were tested. Morphology of the resulting PLA scaffolds was characterized both qualitatively by 3D computed X-ray micro-tomography and quantitatively by mercury porosimetry. Moreover, thermodynamics of the PLA/AA system was characterized both experimentally – by cloud point measurements of binodal curve using thermo-optical measurement (turbidimetry) – and theoretically, by applying Flory-Huggins theory to predict binodal and spinodal curves.

WT/SL41

POZOLAN ACTIVITY OF CALCINED CLAYS AND OTHER POZZOLANS USING THE FRATTINI TEST

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Pozzolans have been used for many decades as an important raw material in construction industry. These are siliceous and aluminum materials which, in the presence of water and calcium hydroxide, are able to form a C-S-H binder phase. C-S-H phase is responsible for the strength of hardened cement. Cement replacement, whether total or partial, has a significant influence on reducing CO_2 emissions, an increasingly discussed topic in recent years. For optimal use of pozzolans, it is necessary to know their reactivity, resp. pozzolanic activity. The aim of the work is to compare the pozzolanic activity for selected pozzolans with a focus on calcined clays, fly ashes and SiO_2 using the Frattini test, resp. according to ČSN EN 196-5.

WT/SL42

REDUCTIVE DEGRADATION OF *M*-TRIFLUOROMETHYLANILINE AND FLUFENAMIC ACID FROM MODEL CONTAMINATED AQUEOUS STREAM

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This lecture is focused on the application and reductive degradation of two CF_3-substituted aromatic compounds – anti-inflammatory drug *N*-(3-[trifluormethyl]phenyl)anthranilic acid (also known as flufenamic acid) and starting material used for the synthesis of the flufenamic acid, *m*-trifluoromethylaniline.

The lecture is structured into two parts. The first part deals with the application of polyfluorinated aromatic compounds and their impact on the environment. Especially the role of flufenamic acid and *m*-trifluoromethylaniline in the production of organic fine chemicals will be discussed and applicable methods for the production of the flufenamic acid will be compared.

The second part of the lecture is focused on the results of the reductive hydrodefluorination of the flufenamic acid and *m*-trifluoromethylaniline in an alkaline aqueous solution. The suitable experimental conditions and chemical agents effective for hydrodefluorination will be presented. The Raney nickel Al-Ni alloy was discovered as an effective reductant for the hydrodefluorination of the flufenamic acid and the *m*-trifluoromethylaniline even at room temperature and ambient pressure. HPLC and GC methods were developed for the quantitative determination of flufenamic acid and *m*-trifluoromethylaniline and their degradation products. The hydrodefluorination of both compounds is compared and the effect of amounts and ratio of Al-Ni and NaOH reagents will be discussed.

WT/SL43

TRIBOELECTRIC SEPARATION OF PLASTIC WASTE AND UTILIZATION OF EXTERNAL ELECTRIC FIELD TO INCREASE ITS EFFICIENCY

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Plastic materials find their use in many applications. This naturally produces large amounts of plastic waste, which accumulate in landfills or oceans. Current recycling methods cannot be widely applied because they are expensive and mostly less environmentally friendly due to the spent energy or used chemicals during the process. Moreover, the wide range of plastic materials makes the universal sorting method impossible, and currently, we are unable to recycle many material mixtures with different physical and chemical properties. Triboelectric separation is a method that utilizes surface properties of materials described, e.g., by work function, to separate materials which broadens the set of separable materials; moreover, it will be cheap and can be automated. This method is based on the phenomenon that each plastic material obtains a different electrostatic charge by friction contact against a proper counter-material. And hereby charged plastic mixture is separated in electric field according to the obtained charge, ergo material. The most important parameter of this apparatus is the changeable counter material, i.e., the material that we rub plastic samples against in order to 'generate' charge. By altering the counter material, we are able to influence the charge of the plastic particles and thus increase the separation efficiency. Additionally, we can assist the charging process with the external electric field by which we can fine-tune the charge on to be separated material and thus to reduce the requirements imposed on the counter-material properties. Using our tribocharging apparatuses, we showed that various plastics could be charged to different saturation charges and, in some cases, even to charge of different polarity. Both purity and yields of sorted material fractions can be further improved by repeated charging and separation cycles.

ABSTRACTS

POSTERS

P01

Heterogeneous Transesterification of Camelina sativa Catalysed by Potassium impregnated Mg/Al Mixed Oxides to prepare Biodiesel

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Mixed oxides obtained from Hydrotalcites provides useful properties in the transesterification reaction [1]. The basic hydrotalcites are composed of Aluminium and Magnesium in cationic layer and different anions mostly CO_3^{2-} or HCO_3^{2-} in interlayer space. Impregnation of Potassium on Hydrotalcite surface could improve catalytic properties, which can cause higher yield of biodiesel from transesterification. As a source of fatty acids Camelina Sativa oil was used. This originally undesirable plant can bloom three times in a year, and it is not demanding in the amount of water, minerals or soil quality.

Mixed oxides were obtained from Hydrotalcites prepared by co-precipitation [2]. Calcinated samples were treated by wet impregnation with solutions of KF, CH3COOK, KNO_3 to improve catalytic activity of mixed oxides. To compare catalyst and their activity, basic properties were measured (XRD, FTIR, TPDA, TPD-CO_2, ICP, SEM). Transesterification was running at temperature of 140 °C (3wt.% of catalyst, molar ratio of Me/Oil 30:1, 7 hours). The content of FAME in the final product was measured by GC analysis [1].

Prepared catalysts were tried in transesterification for FAME production. Basic Mixed oxides without impregnation achieved content higher than 90 wt.% of FAME after 7 hours of reaction. In compared with that, impregnated samples achieved significantly higher number of basic sites and high specific surface area, but content of FAME after 7 hours of reaction was lower than 80 wt.%. The results showed that impregnation of Potassium improved properties of mixed oxides but not catalytic activity.

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P02

COMBINED THERMAL AND CATALYTIC CRACKING OF WASTE PLASTICS IN THE PRESENCE OF CLINOPTILOLITE

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What to do with spent plastics, it is the most important question at present. Their decomposition is too long process because of their durability and the result is their accumulation on landfills. There exist some approaches how to solve this problem. The commonly used method is incineration (energy recovery), but the problem with toxic gases in the air is the result. The other recycling methods as material and feedstock recycling are used also. Feedstock recycling seems to be very promising thanks to the reuse of spent plastics on monomers or valuable fuels.

We studied: the cracking of pure polypropylene without presence and in the presence of origin or acid modified clinoptilolite catalyst, the regeneration and modification of catalyst with goal to produce gaseous and liquid products. Detailed composition of gaseous and liquid products was determined. All experiments were carried out at the same two stage cracking apparatus and at the same reaction conditions. In the first stage the pure polypropylene was cracked thermally. The formed gaseous products were transferred to the second stage, where the cracking in the presence of catalyst was carried out (the case of catalytic cracking). The maximum cracking temperature was 450°C. All experiments were carried out in the inert atmosphere of nitrogen.

The products obtained by cracking were: liquid, gas and solid (in the reactor) and coke (solid residue on the surface of catalyst). The influence of catalyst during cracking was evident. The higher production of gas fraction was observed as a result of cleavage of higher hydrocarbons to smaller. It is thanks to carbenium mechanism, followed by alkylation, polymerization and isomerization reactions. Thermal cracking is other way of cleavage of hydrocarbons. It is a radical mechanism and therefore the production of heavier hydrocarbons was observed (the highest amount of liquid product). It was observed that modification of catalyst has positive influence on gas production also.

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P03

MODELING OXYGEN PRODUCTION VIA CRYOGENIC AIR SEPARATION

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Industrial-scale oxygen production is vital for many industrial branches, where it serves for energy efficient production of materials, as gasification agent or to produce chemicals. Current technologies exhibit a rather large specific power consumption, exceeding 150 kWh per ton of pure oxygen. With several of them being mature for decades, while others being still in development, possibilities for further energy consumption decrease should be exploited, to make the oxygen production via air separation more sustainable. With this long-term goal a model Cryogenic Air Separation Unit (ASU) is considered as a case study. First, its performance as a stand-alone plant is modeled and verified. Second, options for its improvement are identified and discussed. The most feasible option is implemented, and the resulting effects are discussed. Third, possible synergies resulting from its incorporation in a refinery are highlighted, together with the idea of using the oxygen for heavy residues gasification, while nitrogen being supplied to the refinery for inertization purposes. As discussed, deeper energy integration with the refinery energy management could deliver additional power consumption reduction if excess heat from refinery is utilized in the ASU. The presented case study and its result contribute to sustainable industrial-scale oxygen production goal, while retaining a favorable production economy and exploiting the potential of carbon footprint reduction.

P04

ALTERNATIVE USAGE OF MSCR TEST FOR EVALUATION OF TYPE AND CONTENT OF POLYMER IN BITUMINOUS BINDER

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MSCR test is frequently used to assess bitumen resistance to rutting as part of system SUPERPAVE+. The test is designed for evaluation of temporary and permanent deformation during repeated cycles of stress loading and recovery. From the standard evaluation, recovery and non-recoverable compliance are calculated to obtain the supplemental classification of the evaluated bitumen. However, there are alternative approaches for evaluation of MSCR results that may extend the information which is gained from the standard evaluation. In our work, we deal with evaluation of MSCR results using the Burgers viscoelastic model. For samples of bitumen with different composition, the Burgers model is applied on MSCR results. The obtained model parameters are analyzed, in relation to the type and content of polymers that were used for modification.

P05

COMPATIBILITY OF MARINE FUELS CONTAINING ALTERNATIVE MATERIALS

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The implementation of IMO 2020 rules brought a change in the maximum sulfur content in marine fuels on deep seas from 3.5 wt% to 0.5 wt%. There are currently four general ways how to meet the legal requirements. The first one is the continued use of high-sulfur marine fuels in combination with on-board desulphurisation technology (so-called scrubber). The second option is to switch to low-sulfur marine fuels. The third way is the transition to sulfur-free fuel (mainly LNG or hydrogen) and the last option is the usage of alternative low-sulphur materials for the marine fuels production.

However, the persistent problem is still the compatibility of the individual blends. Incompatibilities may occur during the blending of high-sulfur and low-sulfur marine fuels or generally when two or more streams of different origin are blended. The considerations ISO / PAS 23263 has been issued as supplementary material to the ISO 8217 based on new IMO rules. This document provides the guidance for fuel suppliers and users on the quality of new produced low-sulfur marine fuels. The compatibility and subsequent stability of the produced low-sulfur marine fuels can be monitored in addition to ISO 8217 by other complementary methods. These methods include, for example, S-Value, P-value or P-ratio. However, it is necessary to be equipped by very expensive and specific devices to determine these parameters. The big disadvantage of the mentioned methods is their single-purpose use without further alternative application.

For the above-mentioned reasons, the possibility of using alternative raw materials together with quick and simple methods for assessing the undesirable incompatibilities should be considered. The goal of this study was to use the commonly available laboratory methods in the determination of compatibility and stability parameters for laboratory prepared mixtures of standard and alternative streams.

P06

CO-PROCESSING OF PYROLYSIS PRODUCTS

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The current trend of deeper crude oil processing leads to an increase in the use of secondary products for diesel production. One of the possible directions that today's refining industry can utilize is the use of higher generation of biofuels or other materials produced from waste by pyrolysis and their processing into products with higher added value. The problem attached to pyrolysis products are their individual low quality parameters. In particular, the higher amount of sterically hindered sulphur species, nitrogen and aromatic hydrocarbons are observed. For this purpose, the refinery uses a catalytic hydrogenation process during which the heteroatoms of sulphur and nitrogen are removed from feedstock. The addition of alternative pyrolysis products has effects on the most important property (in whole process) the activity of the desulphurisation catalyst. Reduced catalyst activity and the presence of pyrolysis products in feedstock affects the quality of products from catalytic hydrogenation. For this reason, the above-mentioned problematic parameters in products are subsequently detected. Prior to industrial application, the mentioned aspects are usually tested and verified using experimental pilot units. The aim of the experiment is to evaluate the effect of addition of alternative pyrolysis products on catalyst activity and properties of products from catalytic hydrogenation.

We tested the influence of the addition of two alternative pyrolysis products as a component of feedstock processed in the hydrogenation of middle distillates. Specifically, it was a product from the steam cracking of petroleum fractions and product derived from pyrolysis of sorted waste plastic. The influence of each pyrolysis products was tested separately from the other. Influences, advantages and disadvantages of used alternative pyrolysis fractions were described.

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P07

CO-PROCESSING OF ATMOSPHERIC GAS OIL WITH FURFURAL-ACETONE ALDOL CONDENSATION ADDUCTS

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The aldol condensation reaction is an organic synthesis between carbonyl groups at low temperatures (< 100 °C) and atmospheric pressure. This reaction allows the synthesis of platform molecules from furfural and acetone, which are suitable feedstocks for biofuels production.

The hydrodeoxygenation of these furfural-acetone aldol condensation adducts means a valuable catalytic upgrading into n-alkanes in the gasoline or kerosene range. However, the hydrotreating of these compounds over conventional sulfided catalysts (NiMoS/Al_2O_3, CoMoS/Al_2O_3) gives places to a fast catalyst deactivation due to sulfur leaching from the catalyst surface. In this way, the co-processing seems to be a promising alternative route, allowing the hydrotreating of acetone furfural adducts using the existing catalysts and technology.

This study reports the co-processing of atmospheric gasoil, furfural-acetone adducts (5-10%) and isopropanol (co-solvent), using industrial conditions (320 °C, 5.5 MPa, 0.5 h^{-1}) and commercial catalysts for hydrotreating (CoMoS). Our results showed complete conversion of furfural-acetone adducts into n-octane, without a relevant effect on catalyst activity during co-processing.

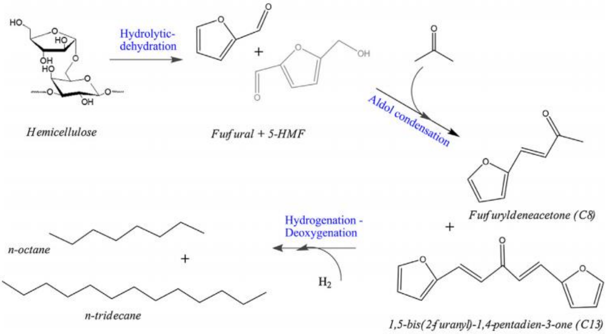

Figure 1. Furtural-acetone aldol condensation and hydrotreating to n-alkanes

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Acknowledgements:

The work is a result of the project which was carried out within the financial support of the Ministry of Industry and Trade of the Czech Republic with institutional support for long-term conceptual development of research organisation. The result was achieved using the infrastructure included in the project Efficient Use of Energy Resources Using Catalytic Processes (LM2018119) which has been financially supported by MEYS within the targeted support of large infrastructures.

P08

HYDROGEN PRODUCTION OPTIMIZATION IN REFINING INDUSTRY

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Considering the current economic and environmental situation in refining industry it is very important to increase crude oil conversion towards more valuable light products. The key factor to deeper conversion is hydrogen, which is mostly produced in refineries by steam reforming technology. These processes belong to most energy consuming, and produce large amount of excess steam, major part of which is usually exported to refinery's steam network. Therefore, right configuration of hydrogen production units' utilization is necessary to reduce refinery's operation costs, to remain competitive in today's fuel market.

SLOVNAFT refinery is relatively small, but complex refinery processing mostly Russian export blend crude oil. Two steam reforming units are currently in operation here, but lately, their maximal hydrogen production capacities are reached more often. It is caused by:

- Decreasing Russian export blend crude oil quality – more hydrogen is used in hydrocracking and desulphurization processes
- Increasing ratio of heavier and sourer feedstock processed in SLOVNAFT refinery
- Continual revamp of existing units to increase crude oil conversion to lighter products and to meet tightening fuel quality standards

Therefore, commissioning of a new hydrogen production unit based on steam reforming is considered in SLOVNAFT refinery.

In this contribution, four investment proposals capable of solving the resulting anticipated steam excess are presented and their impact on steam balance, fuel consumption and electricity production is evaluated.

P09

MUTUAL INTERACTION OF COMPONENTS DURING MEMBRANE SEPARATION OF GASES

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The aim of this study was to demonstrate the mutual interaction of components during multicomponent gas membrane separation. Studied mixture contains CO_2, N_2 and CH_4, the used module was a polyimide hollow-fibre module with 3000 fibres, length 0.290 m and total surface of the fibres 0.820 m^2. The mixture was chosen due to its components having suitable permeabilities in pure form. The permeability of pure CO_2 for the used module is around 342.7 Barrer and the permeabilities of N_2 and CH_4 are very close, being 13.2 and 13.4 Barrer respectively

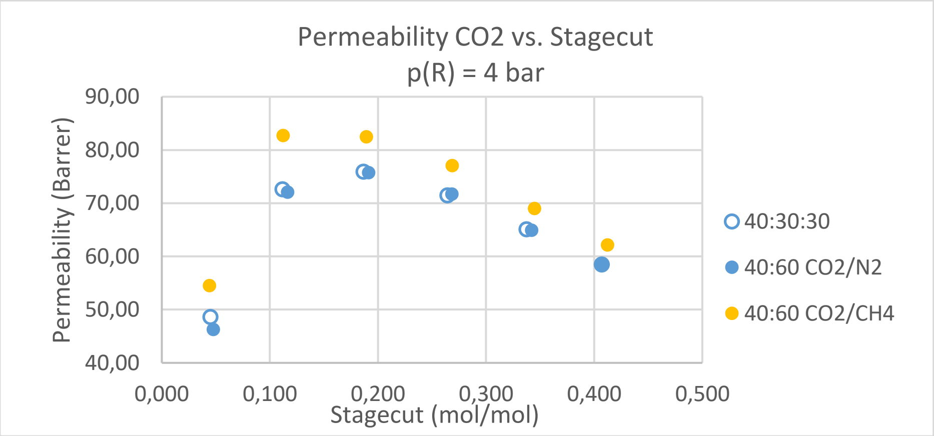

Fig.1: Permeability of CO_2 in three different gas compositions always containing 40 %mol CO_1 with 30 %mol N_2 and 30 %mol CH_4, with 60 %mol N_2 and with 60 %mol CH_4 on molar stage-cut while maintaining

The theoretical selectivity is thus almost identical for CO_2/N_2 and CO_2/CH_4, however the actual selectivities measured differ from each other and from the theoretical ones. Presented data show the shift in permeabilities and selectivities of the components when separated in both binary and a tertiary mixture. Also, possible parameters affecting the process are stated.

Acknowledgements

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P10

INDUSTRIAL COMBINED HEAT AND POWER PLANT REPOWERING PROPOSAL

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Industrial combined heat and power plants (CHP) in Middle Europe face the problem of tightening emission limits and decreasing thermal efficiency resulting from their ageing. At the same time, focus and financial support for renovation activities are directed on ageing thermal power plants nowadays, while the need for revamp of industrial CHPs is a less discussed topic generally. To highlight the need for action in this sector a model case study is presented. It showcases an industrial CHP, fueled with heavy fuel oil, producing steam for industrial use and electricity on a condensing-extraction turbine. Several technologies are considered that could augment its actual performance and lead to cleaner heat and power production. Among those, internal combustion engines (ICE) and gas turbines (GT) are the most frequently applied solutions in scientific studies as well in real repowering activities. Both technologies are suitable for industrial use as well. General features and pros and cons of industrial CHP repowering by those technologies are discussed; system balances are set up and resulting improvement of the repowered CHP is obtained. Energetic, environmental, and economic considerations allow for the most feasible option identification. The actual trend of rising carbon tax is incorporated as well and an extrapolation to 100 € per ton of CO_2 is considered to evaluate the robustness of the best solution.

P11

KATALYTICKÁ METHANIZACE BIOPLYNU S POUŽITÍM KATALYZÁTORŮ NA BÁZI NI A NI/CO

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Jednou z možností snížení emisí oxidu uhličitého při využívání ZP je jeho nahrazení biomethanem, resp. SNG (Sustainable Natural Gas). V tomto ohledu nabývá katalytická methanizace na významu, protože umožnuje efektivně využít přebytků elektrické energie k produkci plynu bohatého na methan. Katalytická methanizace je reakce oxidu uhličitého s vodíkem za vzniku methanu a vody. Vodík využívaný pro reakci lze vyrobit pomocí elektrolýzy vody z přebytků obnovitelné elektrické energie. Zdroje oxidu uhličitého můžou být spaliny fosilních elektráren, oxid uhličitý z průmyslových procesů či ze vzduchu nebo bioplyn.

Katalytická methanizace bioplynu umožnuje jednoduše přeměnit (zušlechtit) bioplyn na biomethan (resp. SNG) bez nutnosti předešlé separace oxidu uhličitého, což zefektivňuje celou výrobu SNG. Další výhodou je i vyšší produkce SNG, protože oxidu uhličitý obsažený v bioplynu je přeměněn na methan. Vyrobený plyn bohatý na methan může být použit například pro pohon vozidel či může být vtlačen do plynárenské infrastruktury a využít její transportní a skladovací kapacitu.

Methan obsažený ve vstupním plynu může za určitých podmínek způsobit deaktivaci katalyzátoru (např. postupné zauhlíkování katalyzátoru). Přítomný methan má také podstatný vliv na teplotu v reaktoru. Tento příspěvek se zabývá vlivem methanu na katalytickou methanizaci za tlaku do 0,1 MPa a teplotách do 520 °C při použití katalyzátorů na bázi Ni a Ni/CO.

P12

BINDING INTERACTIONS OF METYLXANTHINES TO BEECH WOOD

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Methylxanthines are a group of xanthine derivates potentially useful for protecting wood from biological pests. However, nobody studied their interactions with regard to their properties and retention within wood. For this reason, we studied the interactions of caffeine, theophylline, and theobromine with beech wood in the present study. The SEM technique was used to visualize these interactions. The results confirmed the different bonding of the tested methyxanthines to wood. The intensity of binding interactions decreased from caffeine to theobromine. These conclusions are in good agreement with our previous results of biological and chemical studies.

P13

INFLUENCE OF THE ADDITOIN OF BLAST FURNACE SLAG TO ALKALI-ACTIVATED MIXTURES BASED ON NATURAL ZEOLITES

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This study is focused on alkali-activated (AA) materials based on natural zeolites and the mixture of the AA materials and commercial material ZEOSLAG 20, which is a mixture of a blast furnace slag and natural zeolite. The addition of slag to alkali-activated mixtures based on fly ash or metakaolin is used to increase the strength. The increase in strength occurs due to the formation of the CSH phase during the reaction of CaO contained in the slag with silicates in the alkaline activator. The aim of this study was to examine the influence of the addition of blast furnace slag to alkali-activated mixtures based on natural zeolites and observe the effect of subsequent leaching on the properties of these materials. The modification of alkali-activated samples and samples with the addition of slag was carried out by the leaching using 0.1M HCl and then using 3M HCl. Properties of these materials were determined using N_2 physisorption, Hg porosimetry, XRF, XRD, DRIFT and the cutting edge strength measurements. The cutting edge strength measurements showed that the addition of slag to the mixtures had a very significant effect on the strength. The strength of the material increased more than 6 times and decreased only slightly after leaching using 0.1M HCl, while after leaching using 3M HCl there was a significant decrease due to a collapse of the binder CSH phase. The results of N_2 physisorption measurements showed relatively small specific surface areas for unmodified samples (around 30 m^2/g), which by leaching using 3M HCl increased to almost 240 m^2/g. Hg porosimetry showed that the addition of slag reduced the total intrusion volume. Acid leaching using 0.1M HCl and 3M HCl resulted in a slight decrease of the total intrusion volume in all samples. The obtained data showed an improvement in properties and extension of the potential applicability of these materials in the chemical industry especially for catalytic and sorption applications.

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The publication is a result of the project which was carried out within the financial support of the Ministry of Industry and Trade of the Czech Republic with institutional support for long-term conceptual development of research organisation. The result was achieved using the infrastructure included in the project Efficient Use of Energy Resources Using Catalytic Processes (LM2018119) which has been financially supported by MEYS within the targeted support of large infrastructures.

P14

SUBSTITUTED DIPHENYLAMINO STYRYL BENZENES AS PROMISSIVE MATERIALS WITH TUNABLE INTENZIVE SOLID STATE FLUORESCENCE – SYNTHETIC APPROACH TO KEY INTERMEDIATE

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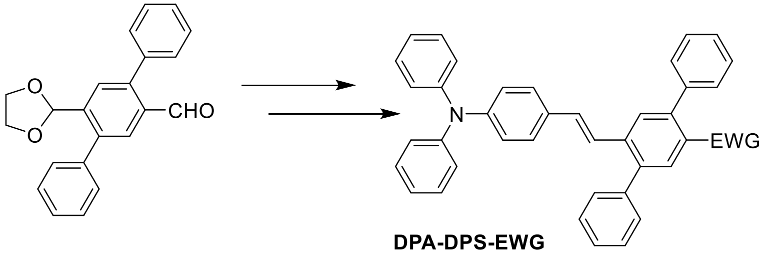
The series of all-trans push-pull end-capped side-diphenyl substituted diphenylamino stylbenes (DPA-DPS-EWG) was prepared by Horner–Wadsworth–Emmons coupling. The important step of synthesis of targeted molecule is preparation of key intermediate: 5'-(1,3-dioxolan-2-yl)-[1,1':4',1''-terphenyl]-2'-carbaldehyde. There are existing several approaches for the synthesis of this molecule. Only some of them bring sufficient result for their synthesis.



In this presentation, we would like to present our approach including unsuccessful experiments, our improvements as well as final experimental approaches to first investigated molecule and at the same time key intermediate for further modifications.

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P15

PRECURSOR-REFORMING SYNTHESIS OF MESOPOROUS g-C_3N_4 NANOSHEETS FOR PHOTOCATALYTIC DESTRUCTION OF ORGANIC DYE AND PHARMACEUTICALS

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Environmental remediation using nanastructered semiconductors with visible light absorption provide an effective way for the removal of emerging wastes. Graphitic carbon nitride (g-C_3N_4) is a subject of the enormous research attention as a promising low cost, visible light driven metal free photocatalyst. However, this π-conjugated polymer semiconductor absorbs light up to 420 nm, posseses high charge separation rate and small specific surface area. The potential applications of g-C_3N_4 in many areas cause the motivation to modulate it's structure and electronic properties to achieve improved implementation. Here we describe a novel precursor reforming strategy that ultimately affords mesoporous g-C_3N_4 materials with red shifted light absorption edge. The precursor synthesis was performed by hydrothermal treatment of mixtures melamine with urea or thiourea. It was confirmed that hydrothermal treatment of melamine and urea (thiourea) causes an irreversible melamine monoclinic to orthorhombic phase transformation. Calcination of the orthorhombic melamine yielded mesoporous g-C_3N_4 with enhanced photoabsorption properties. The structure, morphology and optical properties of obtained g-C_3N_4 were studied with XRD, FT-IR, UV-Vis DRS, N_2 adsorption-desorption methods, photoluminescence and elemental analysis. The synthesized materials demonstrated high photocatalytic activity in degradation under visible light of colored organic dye and colorless antibiotics.

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CZ.02.1.01/0.0/0.0/16_019/0000853 „IET-ER“) and VŠB-TU Ostrava (project No. SP 2021/46)

P16

TIO$_2$-LDH NANOCOMPOSITES FOR ORGANIC DYE REMOVAL FROM AQUEOUS MEDIA BY ADSORPTION AND PHOTOCATALYTIC DEGRADATION

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Layered double hydroxides (LDH) are ionic lamellar compounds known as sorbents, catalysts, anion exchangers, and drug delivery systems. Due to it's unique layered structure, adjustable band gap, large surface area, low cost, and remarkable recyclability LDH attract attention to be applied for the photocatalytic process. The combination of LDH with TiO$_2$ caused the improvement of the photocatalytic activity of hybrid materials. The results on the application of TiO$_2$-ZnCuAl LDH/Ag composites for the removal of the anionic dye Acid Orange 7 (AO7) from aqueous solutions by adsorption and photodecomposition in neutral and alkaline medium will be presented. There was shown that adsorption of AO7 on LDH and its composites with TiO$_2$ can be controllable by pH and by its modification with Ag NP. The highest removal of the dye (99 %) was observed for ZnCuAl MO due to adsorption at pH 7. The photocatalytic degradation of AO7 in the presence of ZnCuAl LDH, its derivatives, and composites with TiO$_2$ was influenced by pH. The activity of all studied materials to degrade dye under UV light greatly increased at pH 11 due to the more efficient formation of hydroxyl radicals. 92 % of AO7 was removed due to the photocatalytic degradation under UV light in the presence of TiO$_2$-ZnCuAl LDH/Ag composites.

P17

VÝVOJ EKOLOGICKÝCH PYROTECHNICKÝCH ZLOŽÍ

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Toxicita chemických látok a ich vplyv na pracovné a životné prostredie je nanajvýš aktuálny vo všetkých priemyselných oblastiach. Vyplýva to z legislatívy v SR a celej EÚ sústavou nariadení, tzv. REACH [1]. Týka sa to aj energetických materiálov (výroba a spracovanie výbušnín). Preto dochádza k náhrade karcinogénnych zložiek a ťažkých kovov, ktoré obsahujú pyrotechnické zlože. Ide hlavne o zlúčeniny bárya, olova, antimónu a ortuti a v menšom množstve aj iných zlúčenín (napr. ZnO, TiO_2).

Vyrábané pyrotechnické zlože sú zavedené od 60. – 70. rokov minulého storočia. Ich najväčším nedostatkom je toxikologická nevhodnosť. Značné množstvo surovín už v súčasnosti nevyhovuje z hľadiska legislatívy alebo končí platnosť výnimiek. Preto je nevyhnutné hľadanie náhrad surovín, resp. návrh a vývoj ekologicky a toxikologicky prijateľných pyrotechnických zloží. Na druhej strane mimoriadne dôležité je, aby nové formulácie mali aj požadované pyrotechnické a výbušninárske vlastnosti, keďže sú súčasťou novovyrábanej munície a muničných elementov. Vyskytujú sa v zapaľovačoch, v iniciátoroch, palníkoch, stopovkách, iniciátoroch, ale aj v civilných aplikáciách – napr. hasiacich zariadeniach, airbagoch.

Práve kvôli dlhodobým zárukám na novú munícíu (až 15 rokov) a prísnym hygienickým podmienkam v civilných aplikáciách, musia byť všetky nové postupy výrob a chemické zloženia prísne a riadne preskúšané.

V rámci projektu *„Ekologicky prijateľné energetické materiály spĺňajúce požiadavky REACH“* podporeného z Európskeho fondu regionálneho rozvoja, spoločnosti ZVS Impex, a. s. Dubnica nad Váhom a STC, s. r. o. Brno ekologizujú aktuálne vyrábané pyrotechnické zlože tak, aby vyhovovali všetkým legislatívnym požiadavkám a zároveň aj náročným pyrotechnickým vlastnostiam.

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P18

CATALYTIC TRANSFORMATIONS OF BIOETHANOL

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Hydrotalcites and other base materials are used as acid scavengers, however their catalytic properties are of importance as well. The idea of transforming ethanol into alkenes and aromatics commenced a century ago, but for decades it has been preferable to produce synthetic ethanol from ethylene. This trend is currently reversed, and bioethanol is becoming a promising raw material for the chemical industry. The introduction of starch-based and in particular cellulose-based processes made ethanol a prospective and economically advantageous raw material. Catalysts play a key role in ethanol transformation, which is a two-step process, where ethanol is converted to acetaldehyde in the first step over a redox catalyst. The second step is catalysed by acid-base catalysts. This step is the most crucial for the formation of the desired unsaturated hydrocarbons. Therefore, we focused on hydrotalcites and zeolites as promising acidobasic catalysts.

We prepared series of heterogeneous catalysts based on sepiolite clay, ZSM-5, BEA, FER, MOR, USY and MCM-22 materials, as well as Mg/Al, Zn/Al, Mg-Ti/Al double layered hydrotalcites. As a reference we used MgO-SiO2 mixed oxides alone or prepared by using ethylene glycol and polyvinylpyrrolidone as pore-forming agents. 2 g of the catalyst was tested in a plug-flow stainless steel reactor with the ethanol load of 5 ml.h-1. 100 ml.min-1 of nitrogen was used as a carrier gas. The gaseous reaction products were analysed using GC, the liquid ones using GC/MS techniques.

Zeolites in H-form promote the dehydration of ethanol in the temperature range 300-550 °C, yielding 21-32 % of ethylene depending on the particular zeolite. Promotion of the zeolites with Ag, and especially Ga resulted in elevated yields of C4 hydrocarbons, which can in turn undergo metathesis reactions, yielding propylene. We achieved a 25.5% yield of propylene using Ga-ZSM-5 catalyst. Doping zeolites with alkaline metals suppressed the dehydration of ethanol. Concerning the liquid products, H-ZSM-5 gives a wide variety of oxygenates and aromatics, while upon doping with Ga, toluene ethylbenzene and xylene are becoming the dominant liquid products. Interestingly, MCM-22-based catalysts promote the formation of alkylnaphtalenes.

Using hydrotalcites as catalysts one can observe a significant effect of the Mg/Al molar ratio during the synthesis of the hydrotalcites; decreasing this ratio from 3 to 0.5, the 1,3-butadiene yield increases from 7.9 to 37.4%. Doping hydrotalcites with Ti increases the yields of acetaldehyde to 43.7%. The conversion of these high yields of acetaldehyde to the most desired 1,3-butadiene is a subject of further research.

Acknowledgement:

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P19

CATALYTIC OXIDATION OF FURFURAL TO MALEIC ACID IN THE PRESENCE OF IRON BASED CATALYSTS

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Furfural is a C_5 compound produced from hemicelluloses by dehydration in acidic media[1]. Selective oxidation of biomass based furfural to maleic acid or maleic anhydride which are currently produced from benzene and/or butane is an alternative route to the on-going fossil base processes. Oxidation of furfural in both vapor and liquid phases using various types of metal catalysts have been studied[2,3,4]. The recent developments in maleic acid synthesis from bio-derived chemicals over homogeneous or heterogeneous catalysts were summarized lately in review paper[5].

In the present work, new type of heterogeneous catalysts have been explored to convert furfural in aqueous phase to maleic acid. Several iron phosphate type catalysts were prepared by coprecipitation at different atomic ratios of precursors and subsequent calcination. For comparison, also another types of iron catalysts were tested. Oxidation reactions were carried out in 10 mL stainless steel autoclaves lined with glass mainly at the temperature of 120 °C and oxygen pressure 0.8 MPa during 18 hours. The liquid samples were analyzed by high performance liquid chromatography equipped with UV and RID detectors, using a HPX-87H column and 5 mmol L^{-1} sulfuric acid aqueous solution as the mobile phase.

The highest yield of maleic acid (22,1 %) as the desired reaction product at 89,4 % conversion of furfural was achieved using the $Fe_2P_2O_7$ catalyst prepared at the atomic ratio of precursors Fe:P = 1 and calcined at the temperature of 600 °C.

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P20

EFFECT OF THE SUPPORT ON MANGANESE CARBON CATALYSTS FOR OXIDATION OF CYCLOHEXANONE BY MOLECULAR OXYGEN

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Carbon materials have an increasing number of applications in catalysis, either as catalysts, or as supports for active phases. The nature and concentration of surface functional groups of carbon materials may be modified by suitable thermal and/or chemical post-treatments[1]. The catalytic performance of Mn-based carbon catalysts in the liquid phase oxidation of cyclohexanone with molecular oxygen in the solvent-free system was studied. The influence of carbon supports and preparation conditions on carbon based catalyst activity and selectivity to adipic acid as well as diacids with smaller carbon chains, e.g. glutaric acid and succinic acid, were evaluated from reaction tests. Commercial carbons activated charcoal Norit (Fluka) and carbon black Vulcan XC-72 (Cabot) were demineralized and thermally treated in nitrogen flow. Carbon supported manganese catalysts were prepared by the wet impregnation method described in the paper[2]. The nominal weight loading of manganese was 1 %. The oxidation experiments were carried out in a stirred batch reactor with equipment for monitoring of oxygen consumption at temperature between 80 – 120 °C and the pressure of 0.35 MPa. The reaction mixture was analyzed by gas chromatography. The treatment of activated charcoal Norit at different temperatures strongly influenced the conversion of cyclohexanone and selectivity to diacids. The thermal treatment of active carbon reduces the amount of acidic groups present on its surface and create basic groups such a pyrone type what is in agreement with literature information[3]. Addition of manganese to activated charcoal Norit treated in nitrogen at 900 °C caused a decrease in the catalytic activity and had only minor effect on the adipic acid formation compared to the pure Norit catalysts. On the other hand, adding Mn to demineralized carbon black Vulcan greatly enhanced the reaction rate and formation of adipic acid. A significant influence of reaction temperature and manganese precursor on the oxidation of cyclohexanone over Mn based carbon black Vulcan catalyst was observed. A drawback of Mn supported catalysts on carbon is leaching of metal what is reflected by decreasing in the reaction rate in catalytic tests with a recycled catalyst.

Acknowledgement:
This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-17-0302.

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P21

PREPARATION OF PSEUDOPEPTIDE ALDEHYDES AND VINYL SULFONES AS A POTENCIONAL PROTEASOME INHIBITORS

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Proteasome is 2,5 MDa large multi-subunit complex responsible for the protein degradation in cells. Inhibition of this process is one of strategies for suppression of uncontrolled proliferation of multiple myeloma or leukemia cancer cell lines.[1] We developed novel *O*-benzyl salicylamide-based inhibitors built from leucine and phenylalanine with nanomolar antiproteasomal activity.[2, 3]

To follow our studies we synthetized and fully characterized a new series of *O*-benzylsalicylamides having tripeptide chain containing optically pure aminoacids (*L*-Leu, *L*-Trp, *L*-NLeu, *L*-CHA, *L*-Pro, *L*-Phe) and terminated with aldehyde or vinyl sulfone warhead. All novel salicylamides were tested for their antiproliferative properties against various cancer cell lines derived from hematopoietic malignancies and the resulting data will be presented.

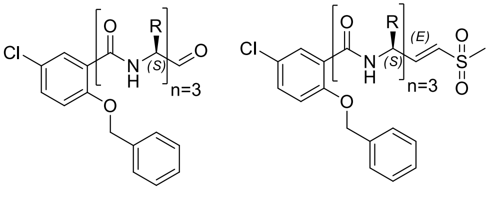

Fig.1: General structures of novel tripeptidic aldehydes and vinyl sulfones

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P22

SELECTIVE MEERWEIN-PONNDORF-VERLEY REDUCTION OF CINNAMALDEHYDE OVER AL-CONTAINING CATALYSTS

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Cinnamyl alcohol, the desired compound with large utilization in the perfume industry due to its properties, can be prepared from cinnamaldehyde by the selective hydrogenation of a carbonyl group keeping C=C bond. An alternative way to prepare cinnamyl alcohol is offered by the Meerwein-Ponndorf-Verley (MPV) reduction, which is less demanding to the catalyst and conditions. Industrially, the most often used catalyst is aluminium-2-propoxide [1] and propan-2-ol as a hydrogen donor. The use of aluminium 2-propoxide, however, requires the addition of high excess of this catalyst to obtain acceptable yields. Based on the literature overview, MPV reduction could be catalyzed heterogeneously as well to avoid difficult, costly and time-consuming elimination of homogeneous catalysts. This work focuses on the utilization of solid Al-containing catalysts such as commercial alumina CG-20, acid-activated alumina I 504 C, laboratory prepared acid-activated alumina, MCM-41, layered double hydroxides, and mixed oxides and their possible recovery and reuse. Using laboratory prepared acid-activated alumina approx. 70% conversion with 70% selectivity to desired cinnamyl alcohol was achieved after 12 hrs of reaction. Acid activated alumina was recycled 3 times. The conversion achieved after 3 hrs of reaction decreased from 56 to 46 %, the selectivity remained at approx. 70 %.

P23

THE EFFECT OF TEMPERATURE AND CONCENTRATION OF WATER ON OXIDATION OF DICYCLOHEXYLAMINE WITH AIR

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Dicyclohexylamine is mostly produced by gas-phase hydrogenation of aniline or disproportionation of cyclohexylamine over a nickel catalysts. During the storage of this amine in stainless steel barrels, its quality decreases due to the contact with the air atmosphere, leading to increase in the concentration of contaminants, especially *N*-cyclohexylidenecyclohexanamine (NCCHA). This work deals with the study of the effect of temperature and concentration of water in dicyclohexylamine on the reaction rate of its homogeneous non-catalyzed oxidation to its imine, NCCHA, with air. The experiments were carried at temperature 50-100 °C and 0.04-0.60 wt. % of water. At the reaction temperature range 50-60 °C and time of experiment 7 h, an increase in the concentration of abovementioned product was not observed. At the 70-100 °C the concentration of main product increased linearly, howbeit, due to the consecution reaction, i.e. its hydrolysis to cyclohexylamine and cyclohexanone, its concentration became stagnant. It was observed that the reaction rate was accelerated by the higher concentration of water. Furthermore, with the increasing concentration of water to 0.60 wt. % in dicyclohexylamine, the rate of the hydrolysis of NCCHA to cyclohexylamine and cyclohexanone increases almost ten times.

P24

A COMPARATIVE STUDY OF DIFFERENT POLYMER MATRIX WITH PHOTOACTIVE PIGMENT ON THERMAL AND ANTIBACTERIAL PROPERTIES

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This study is focused on the preparation and characterization of three different polymer matrices (PA, PET, and PLA) dyed in mass with 0.5 wt% of photoactive pigment. The samples were prepared by the thermoplastic process by the twin-screw extruder and press molder. It is known that a matter of importance regarding particulate samples is the interface between the additive and the matrix in addition to their distribution in, dispersion in, and interfacial adhesion with a polymer matrix. Hence, the observation was made herein of the microstructures of the cry-fractured samples by scanning electron microscopy to investigate the morphology and homogeneity of the prepared samples. Thermal properties of films were examined using differential scanning calorimetry and thermogravimetric analysis. The effect of polymer matrix on antibacterial activity of prepared films was studied according to the ISO 22196:2011 standard. This work shows the differences in the thermal properties for all studied types of polymers with the absence/presence of dye in the matter. Moreover, it describes the polymer matrix influences on the antibacterial activity of the surface of the dyed polymer films. The obtained results indicate that it is possible to prepare formulation as a promising alternative platform in the selective antibacterial treatment of polymer surfaces using perylene-based dyes.

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P25

SWELLING PROPERTIES AND BIODEGRADABILITY OF A NEW AGRO-HYDROGEL BASED ON RENEWABLE MATERIALS FOR AGRICULTURAL USE

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This work describes a new type of renewable and biodegradable hydrogel based on a by-product of dairy industry - acid whey and cellulose derivatives (carboxymethylcellulose and hydroxyethylcellulose) crosslinked with citric acid for application in agriculture as a soil conditioner. The whey as a main component of the hydrogel, might also act as a nutritive agent for boosting the growth and quality of crops due to the high content of organic compounds present in the whey. The water holding capacity, water re-absorption and water retention behaviour of hydrogel in soil were evaluated. The course of biodegradation of the hydrogel in soil was monitored by the measuring of weight loss and quantified by the detecting and measuring the production of carbon dioxide through analysis of the gaseous phase by gas chromatography. Changes in the chemical structure and morphology of the hydrogels during biodegradation were assessed by Fourier transform infrared spectroscopy and scanning electron microscopy. The novel hydrogel demonstrates a high capacity for water absorption and exhibits pH-dependent swelling behaviour with a swelling ratio exceeding 1600% making it comparable with commercially available products. Moreover, the hydrogel has good re-swelling ability and water uptake sustainability in soil after four swelling-drying cycles. The hydrogel is highly biodegradable in soil, since most of its compounds are easily mineralized by microorganisms when biodegradation commences. The stability of the hydrogel in the soil was enhanced by the presence of citric acid, due to the cross-linking reaction between carboxylic groups of cellulose derivatives. This makes citric acid a suitable alternative to synthetic acrylic acid. In summary, the novel agro-hydrogel is a promising material for agricultural use, especially for controlled moisturizing to improve water holding capacity of soil and for nutrient release.

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P26

TWO STAGE CATALYTIC CRACKING OF HDPE AND PP IN THE PRESENCE OF NATURAL AND SYNTHETIC ZEOLITES

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Plastic are very versatile materials, therefore they can be applied in households as also in industry. The problem is the production of plastic waste, because of its long degradation on landfills, which has negative impact on environment. Dominant plastics in the plastic waste are polypropylene and polyethylene. Therefore, our study was to aimed on degradation of these two types of plastics.

The influence of the catalysts on the amount and composition of gaseous products during the decomposition of pure polypropylene and polyethylene in a two-stage reaction system consisting of semi-flow reactor in the first stage and of flow reactor in the second stage was monitored. The effect of natural zeolite clinoptilolite and synthetic zeolite HZSM-5 (extruded alumina and HZSM-5 in ratio 1:1) was tested. With aim to determine cracking activity of catalysts also the thermal cracking was carried out.

Following experiments were performed: thermal cracking, catalytic cracking in the presence of clinoptilolite in the first stage and catalytic cracking in the presence of zeolite HZSM-5 in the second stage. From the results it is evident that the addition of the catalysts to the reaction system produces a higher amount of the gas fraction. The significant influence on the formation and composition of gaseous fraction has synthetic zeolite HZSM-5 for both polymers. It is reflected on the highest yields of the gas fraction: 61% for PP and 63% for HDPE. It is 3.3 times more (PP) and 3.2 times more (HDPE) as was obtained from thermal cracking. Thanks to the presence of HZSM-5 the content of linear hydrocarbons in the liquid fraction of HDPE decreased and the production of aromatic hydrocarbons increased. The aromatic content increased also for PP.

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P27

AMINE-FUNCTIONALIZED POROUS POLYMERS FOR SELECTIVE CO_2 ADSORPTION

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Porous materials have always attracted high scientific interest because of their outstanding performance and potential applications in various fields, including adsorption and gas separation. Hyper-crosslinked polymers (HCPs) have several advantages over other porous materials, they show extremely high surface areas and porosity, low density, outstanding adsorption properties, high chemical, and thermal stability.

Herein, we reported a synthesis, characterization, and the CO_2 (and other gases) adsorption performance of series of novel styrene-divinylbenzene based HCPs. The material was prepared in two steps. The first step involved the radical copolymerization of divinylbenzene (DVB) and 4-vinylbenzyl chloride (VBC), under solvothermal condition to generate porous polymers with high surface area above 700 $m^2 g^{-1}$. In the second step, various polyamine species were applied to react with the alkyl chloride groups and functionalize the pore surface to improve the CO_2/N_2 and CO_2/CH_4 selectivity.

Acknowledgement

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P28

LIMITS AND BARRIERS TO PRODUCT LIFE CYCLE MONITORING FOR CHEMICALS – A CASE STUDY

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Monitoring the product life cycle and the introduction of the eco-design principle is a prerequisite for the effective implementation and enforcement of the circular economy concept. The presented paper focuses on the issue of the possibility of monitoring the life cycle of chemicals with emphasis on the ability to monitor chemicals in the value chain. Finding out the possibilities of life cycle monitoring of a selected chemical substance – basic inorganic acids – are presented and the limitations and limits of life cycle monitoring of chemical substances for the needs of the circular economy are discussed.

P29

GREEN HUMAN RESOURCE MANAGEMENT IN COMPANIES OF CZECH CHEMICAL INDUSTRY

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Green human resource management (Green HRM) includes specific HR policies and procedures in compliance with the three sustainability pillars – environmental, social, and economic. Successful implementation of sustainable corporate strategies in the social, economic, and environmental areas requires clear definition of the means and processes that could be supportive of it. Success of these measures depends, to a considerable extent, on the employees and their so-called green behaviour. Most employees feel co-responsible for the environment and show stronger determination, job satisfaction, and loyalty to employers going a "green way" and taking an active part in support of the environment. As a result, Green HRM can help companies implement measures decreasing the environmental impacts more easily, decrease the environmental devastation in general, or, on the other hand, improve the environment with significant assistance from educated and active employees.

This paper focusses on chemical companies and emphasises the irreplaceable role of their HR in implementation of Green HRM procedures and principles. The research was aimed at the environmental pillar of Green HRM and examined its fulfilment in the practice of chemical companies in the Czech Republic. The paper aims to identify the rate of incorporation of Green HRM-oriented activities into the main corporate HR activities - recruitment and selection of new employees who are more responsible towards green business practices, stimulation of employees to accept environmental procedures for greener business, education for a responsible approach, bonus allocation, and implementation of some initiatives for human resources. The research was conducted through a questionnaire, where the respondents were HR managers of the selected chemical companies in the Czech Republic.

P30

SUSTAINABLE PACKAGING INNOVATIONS FOR COSMETIC PRODUCTS

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Most packaging material flows for consumer chemicals are linear in nature. The packaging in these flows is made from primary raw materials for single use and ends up in a landfill or incinerator at the end of its life cycle, which has significant impacts on the environment, society and the economy. In order to increase the sustainability of packaging, researchers are currently focusing on the concept of circular economics, in which material flows are closed into functional and endless cycles. The aim of the paper is to identify sustainable packaging innovations that are based on the principles of circular economics. Qualitative research was carried out at two manufacturers of cosmetic products (surfactants and creams) using the method of semi-structured interviews. The content analysis of interviews from both companies and their subsequent synthesis identified opportunities for sustainable innovations of primary packaging for cosmetic products, namely in the areas of reducing, reusing and recycling of packaging materials. The results of the research not only contribute to theoretical knowledge in the field of sustainable packaging innovations, but can also help companies in the chemical industry to decide on an innovation strategy in the field of primary packaging.

P31

IDENTIFIKACE FAKTORŮ OVLIVŇUJÍCÍCH CENY ROPY A ZEMNÍHO PLYNU A JEJICH VZÁJEMNÉ KORELACE

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Trh s ropou a zemním plynem je pod vládou cenové volatility a nejistoty. Mezi významné vlivy, které potlačují nebo naopak umocňují nejistotu a volatilitu, lze zařadit omezování produkce významných těžařů, rostoucí počet aktivních vrtů ve Spojených státech amerických, apod.

Cílem příspěvku je identifikovat relevantní faktory ovlivňující ceny komodit, a to ropy a zemního plynu. K tomu účelu bude využit matematicko-statistický aparát v podobě nástroje vícenásobné regresní a korelační analýzy. Vybrané nástroje nám umožní kvantifikovat síly jednotlivých závislostí a bude možné na stanovené hladině významnosti verifikovat relevantní faktory popisující chování cen obou komodit. Vstupní faktory budou vybrány na základě ekonomické relevance. Budeme uvažovat i vliv současné pandemie COVID-19. Výstupem předkládaného článku bude, že ze sestavené množiny vstupních faktorů se pomocí vybraných nástrojů vícerozměrné regrese a korelace rozdělí na dvě skupiny. První skupinu budou tvořit faktory, které nebudou mít žádnou souvislost s cenou ropy či zemního plynu, a druhou skupinu budou tvořit faktory ovlivňující cenu ropy či zemního plynu. Dalším výstupem tohoto příspěvku bude komparace citlivostní analýzy modelu popisující cenový vývoj ropy s citlivostní analýzou modelu popisujícího cenový vývoj zemního plynu.

P32

PREPARATION OF MELOXICAM INTERACTIVE POWDER MIXTURES BY MIXING AND CO-MILLING: SURFACE ENERGY AND DISSOLUTION RATE STUDY

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Insufficient water solubility of a drug limits its bioavailability after oral administration. Therefore, improving dissolution rate is one of the major challenges for pharmaceutical research. A natural polysaccharide chitosan (CH) is introduced in this work as a carrier to prepare binary interactive mixtures in order to enhance the dissolution rate of meloxicam (MX), a model Biopharmaceutical Classification System (BCS) II drug. The interactive powder mixtures were prepared in three different drug/excipient mass ratios 1:1, 1:4 and 1:8 using physical mixing or solventless co-milling (planetary ball mill). A flow-through dissolution apparatus (USP 4, phosphate buffer pH 6.8) with open loop equipped with a powder cell was used to evaluate the relative drug dissolution rate r_{rel} (min^{-1}) . The specific surface area S_{BET} (m^2/g) was evaluated according BET theory using nitrogen adsorption (Gemini VII 2390, Micromeritics, USA). Surface energy γ ($\mathrm{mJ\ m}^{-2}$) (IGS/SEA, Surface Measurement Systems, Ltd., UK) was determined using non-polar and polar probes, respectively. A constant sample surface coverage (5 %) and carrier gas (helium) flow rate of 10 mL/min were used. The results confirmed that the mixing as well as the milling with CH increased the dissolution rate r_{rel} (min^{-1}) of MX significantly. The highest maximum relative dissolution rate of meloxicam r_{MAX} 0.50 min^{-1} was detected for the MX-CH 1:8 mixture co-milled for 30 minutes which was five times higher compared with the corresponding physical mixture. The hypothesis that chitosan acts as a suitable carrier in the co-milling process was demonstrated by correlation analysis. The specific surface area of the mixture as well as its total amount (i.e. the total surface) are the controlling parameters of the dissolution rate. Finally, the balance of the cohesive and adhesive forces ($W_{\mathrm{adh}}/W_{\mathrm{coh}}$ ratio) close to one encourages the conclusion about the successful production of MX-CH interactive mixtures.

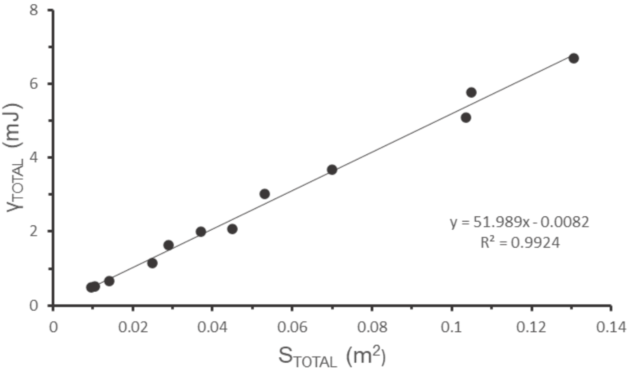

Figure 1. Correlation between total surface energy of the system γ_{TOTAL} (mJ) and total surface area S_{TOTAL} (m^2) for all studied samples.

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P33

A STEREOSELECTIVE STUDY OF ALFAPROSTOL OMEGA CHAIN SYNTHESIS - APPLICATION POSSIBILITIES IN THE SYNTHESIS OF INTERMEDIATES

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Prostaglandins (PG) a well known compounds are a group of lipid mediators with multiple pharmaceutical and veterinary applications. These compounds also bring a significant economic effect to their producers. Synthesis of these compounds is performed by using old protocols with multistep reaction procedures.[1] For this reason, we investigated a several possibilities of synthetic Prostaglandin F2α methyl ester analogue – Alfaprostol. This molecule contains, in comparison with other PG, propargyl moiety in omega chain. This moiety is well discussed in literature. Over past decade a huge number of studies described formation of propargyl moiety with or without stereospecific aspects of this reaction were described.[2] For this reason, we investigated this reaction in lab scale and further on its possibility to apply in chemical industry.
Classical approach to Alfaprostol omega chain (literature) and our novel methodology for this organic specialties will be discussed.

Acknowledgements: the authors wish to acknowledge the financial support of the Faculty of Chemical Technology, University of Pardubice as well as to the Cayman Pharma Neratovice (Czech Republic) for cooperation.

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P34

DISSOLUTION KINETICS OF COMMERCIALLY AVAILABLE TABLETS USING AN OPTICAL MICROSCOPY TECHNIQUE

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Nowadays available commercial products often show poor solubility in water, which leads to problems with achieving proper drug concentration in the patient’s body. One of the limiting factors is disintegration speed. Slow disintegration process will hinder subsequent dissolution process necessary to reach and maintain that concentration. Disintegration is quite complex process and involves liquid penetration and fragmentation of the tablet. To precisely describe it requires using more than a pharmacopoeial method. Several methods offer different options to closely monitor specific parts of the disintegration process. One of the possible methods is optical microscopy. This allows quite precise monitoring of an initial fragmentation during the disintegration process, since the released fragments are not subjected to any outer force and can be analysed in their true size, unlike using methods where a stirrer is used to keep the fragments from sedimentation during the measuring process (e.g. static light scattering).

This paper describes a use of optical microscope as a method for monitoring fragment populations released from tablets of two commercially available drugs containing the same API (ibuprofen). Both formulations were tested in different media and their disintegration kinetics are compared with the results from another method using a static light scattering. This allows to evaluate possible differences in the results of these two methods, and it can help further understand the disintegration process as a whole and potentially improve certain disadvantages of the static light scattering method. For each formulation, the tablet was placed into a small volume of tested medium, and after certain amount of time placed under optical microscope to obtain PSD using image analysis. The key parameters of disintegration kinetics were estimated using erosion-fragmentation regression model. The deeper and more precise knowledge of the disintegration process associated with poorly soluble drugs can help to identify the rate-controlling step of their release and to find proper measures for improving their dissolution rate. Moreover, it can be used to help develop generics with more desirable dissolution profiles, thus making the potential drug more interesting for the manufacturer or the patient.

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P35

MONITORING THE ROLL COMPACTION PROCESS VIA RIBBON STIFFNESS MEASUREMENT

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Typical industrial development of a roller compaction process includes changes in scale from laboratory to pilot, and then further to production scale and also transfer to different equipment designs due to equipment availability in different manufacturing facilities. Different equipment designs, such as feeding system, side seals, roll width or surface, and ribbon milling systems, as well as the process control regime can lead to changes in downstream quality attributes, including granules and tablets. The objective of this work was to monitor the process performance by measurement of compacted ribbon properties using the texture analysis.

The compactors [Alexanderwerk AG, Germany] and [Gerteis Maschinen and Processengineering AG, Switzerland] were used for this study. They have the roll force control using a hydraulic pressure system, but they differ in raw material loading, roll width, and roll diameter. The formulation comprising the atorvastatin API and calcium carbonate, as major excipient was used as the model mixture.

The production was carried out following a common design of experiments in which three levels of pressure or compaction force were measured on each compactor. The gap width, roll/screw/sieve speed were also investigated. The ribbons taken out from the compaction process were collected and characterized by compression test method using CTX Texture Analyzer [AMETEK Brookfield, USA]. While the ribbon compression testing with blade probe did not provide results reflecting the state of compaction, the compression testing with needle probe allowed to measure relative ribbon stiffness, which correlated with the compaction pressure and reflected the local ribbon properties.

The measured relative ribbon stiffness was used to evaluate ribbon uniformity and compare the performance of different compaction equipment. It was found the Alexanderwerk facility exhibit lower lateral ribbon uniformity leaving a large amount of uncompacted material compared to Gerteis. The uneven filling of the gap in the lateral direction of for the Alexanderwerk compactor is the likely cause. The instrumented method of monitoring the product quality can be further used for optimizing the process parameters and technology transfer between the different manufacturing facilities.

P36

TECHNIQUE OF PHARMACEUTICAL POWDER COMPRESSIBILITY MEASUREMENT FOR UTILIZATION IN PREDICTIVE MATHEMATICAL MODELLING OF COMPACTION PROCESSES

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Mathematical modelling of pharmaceutical operations requires fundamental data, covering the process from many aspects and roller compaction of pharmaceutical mixtures is not an exception to this practice. Rheological and mechanical properties of the pharmaceutical powders must be accurately determined for practical application in the modelling of this process. In this work we present a method to determine compressibility for application in mathematical modelling of roller compaction. Compressibility is a mechanical property of powders that describes the volume reduction of a bulk powder when subjected to compaction pressure. It is used in mathematical modelling to predict the extent of compaction, which governs the final apparent density of the compact. The method presented is based on practical implementation of Johanson's compressibility model (1965) and was executed using a uniaxial compression machine that records applied load on the material and displacement of the punch to determine compressibility. The applicability of this approach was demonstrated on model and real pharmaceutical mixtures. The measured values of compressibility for these mixtures were used in mathematical modelling to predict the final apparent densities for their compacts.

P37

PET-G as a PET contaminant

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Currently, PET bottles' recyclers are increasingly confronted with a new type of contaminant - PET-G, which began to be used as an alternative to PVC. The group of copolymers referred to as "PET-G" is extensive and contains more than 60 modifications. They differ in the molar ratios of the copolymer's components, which fundamentally affect the physical properties. The final products are commonly referred to as "PET". PET-G is therefore often perceived only as another PET type.

Although PET and PET-G physicochemically similar, PET-G has a mainly different melting point. Therefore, in some countries, PET-G has been excluded from recycling category 1 (PET) and classified in category 7 (other plastics). Opponents of this reclassification argue that it is sufficient to adjust the sorting devices' sensitivity with NIR detectors.

In our analysis, several dozen samples, which the recycler identified as contaminants, were examined to detect the presence of PET-G. Because there is no standard for PET-G, two products for 3D printing were used, declared by the manufacturer as "PET-G".

According to our results, one of the PET-G samples corresponds with the PET standard. On the contrary, the second shows significantly different thermophysical properties. The difference is also confirmed by FITR-ATR analysis.

More than half of the total amount of contaminants analyzed corresponds to this type and can be identified as "PET-G". This type of PET-G is, therefore, significant contaminant of recycled PET. However, identification is possible only due to a few characteristic peaks of the spectrum. The agreement of whole spectra exceeds 95%.

FTIR is more sensitive than industrial NIR detectors. Thus, it is unlikely that PET-G can be separated from PET by simply adjusting the NIR detectors' sensitivity.

The aim of this paper is, therefore, to point out the problem of using PET-G.

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P38

MODELLING PARTICLE SIZE CHARACTERISTICS AND SPECIFIC ENERGY DEMAND FOR KNIFE-MILLED BEECH CHIPS AT DIFFERENT MOISTURES

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Biomass size reduction technology belongs among the crucial steps being always found at biomass to "X" conversion technologies. This size reduction step is a costly operation that consumes about 33% of the total electrical demand. Thus reducing the energy requirement and the right solution for grinding or milling of biomass would improve the whole process economics. The contribution aims to define a model predicting particle size characteristics and energy demand for knife milled beech chips of different moistures on machine variables.

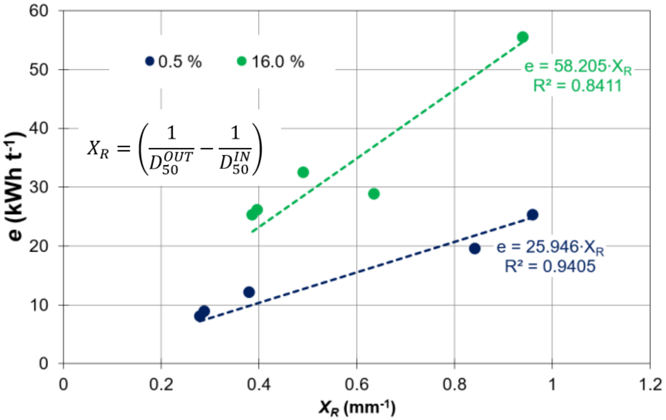

Fig.1: Specific energy demand in dependence on particle size characteristic X_R at given moistures (point – experimental value, curve – regression model).

The experiments were conducted for beech chips of moisture being 0.5, 7.5, 16.0 wt % dry mass, single blade rotor with the constant peripheral speed of revolution being 10.2 m s^{-1} (1500 min^{-1}). The preliminary results evinced that particle size distribution and specific energy requirement are significantly affected by biomass moisture, see Fig. 1. It was found that beech chips of moisture 0.5 - 16.0 wt % dry mass evinces brittle behaviour. Thus, the Rittinger comminution law was an applicable model to predict the energy requirement of size reduction with Rittinger's constant dependence on biomass moisture.

Acknowledgements

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P39

RESOURCE RECOVERY FROM WASTE POLYSTYRENE VIA THERMO-CATALYTIC DEPOLYMERIZATION

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Polystyrene (PS) is the fourth-most abundantly produced commodity plastic. It is widely used in packaging, construction, electrical and electronics and medical equipment, and consequently a large amount of PS waste is generated. Due to poor plastic recycling rates globally, a large amount of plastic waste ends up in the oceans and landfills, posing serious threats to human and animal health and the environment. Chemical or feedstock recycling is considered as an environmentally friendly approach which can be used for the treatment of waste plastics. With this approach, waste polymeric materials can be converted into their original monomers and other valuable chemicals. Chemical recycling of waste polymeric materials can be realized by thermal or thermo-catalytic depolymerization. In this regard, for an enhanced resource recovery, reactor configuration and operating conditions can play important roles. Recently, we have investigated the influence of operating conditions and reactor configuration on the product distribution in the pyrolysis of pure PS. The present work deals with the thermo-catalytic depolymerization of waste PS using the operating conditions that were determined in our previous work. The waste PS materials used as feedstocks were obtained from toner cartridge and from recycled PS of the type HIPS (high impact polystyrene). The pyrolysis experiments were performed in a lab-scale test trig with a horizontal tube reactor heated with a cylindrical heating jacket. The pyrolysis oil was analyzed using a GC-MS system. The influence of operating conditions on the product distribution as observed in the case of pure PS was confirmed for PS wastes also. Furthermore, it was demonstrated that the product distribution also depends on the type of PS feedstock used. This may be ascribed to the catalytic effects of some additives present in different PS materials.

P40

ODOLNOST SMĚSÍ Z ČESKÝCH VYSOKOTEPLOTNÍCH POPÍLKŮ VŮČI STŘÍDAVÉMU ZMRAZOVÁNÍ A ROZTÁVÁNÍ

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Vysokoteplotní hnědouhelné popílky z českých elektráren a tepláren patří mezi cenné druhotné suroviny používané ve stavebnictví. Jejich použitím jako příměsi do cementů se snižuje spotřeba primárních surovin a množství emisí CO_2 vznikajících při výrobě nového slínku. Tím se využití těchto popílků stává jak ekonomicky, tak ekologicky přínosné. Cílem práce bylo pomocí mrazové zkoušky ověřit využitelnost vysokoteplotních elektrárenských popílků odlišného původu jako příměsi do cementu. Byla připravena řada směsí kaší obsahující 75 % cementu a 25 % popílku různého původu, konkrétně z elektráren Počerady, Tušimice, Prunéřov či z teplárny Dvůr Králové. Poté byly připraveny kaše z popílku z elektrárny Tušimice s obsahem 15 % a 35 %. Všechny směsi byly umíchány s ohledem na optimální množství provzdušnění 4-7 % pomocí tlakoměrné metody ČSN EN 12350-7. Dále byly připraveny dvě směsi z popílku z elektrárny Tušimice s provzdušněním 2 % a 9 %. Po 28 dnech zrání ve vlhku byly směsi podrobeny zkoušce střídavého zmrazování a roztávání v prostředí H_2O a 3 % NaCl, přičemž byla zkoumána odolnost jejich povrchu ve smyslu normy ČSN 73 1326, ZMĚNA Z1.

P41

PHOTOCATALYTIC DECOMPOSITION OF NITROUS OXIDE OVER SULPHUR MODIFIED GRAPHITIC CARBON NITRIDE

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Graphitic carbon nitride (CN) is one of the very promising metal-free photocatalysts with semiconducting properties that has been intensively studied during the last decade. Its important physico-chemical properties are high thermal, physical, and photochemical stability. CN absorbs visible light as a result of the band gap energy of ca. 2.7 eV. CN can be prepared by physical or chemical vapour deposition (PVD, CVD) but bulk synthesis from simple precursors by methods focused on the thermal condensation of nitrogen-rich precursors, such as cyanamide, dicyandiamide, melamine and so forth allows for high production at a low cost. However, in as-prepared state, it suffers from certain disadvantages, such as namely low specific surface area and fast recombination of photoinduced electron – hole pairs. They can be can be overcome by exfoliation and doping, for instance, with non-metal elements, such as sulphur, phosphorus, nitrogen and oxygen.

In this work, the doping of CN with sulphur based on the direct synthesis from thiourea (S-CN) and the modification of the prepared CN with mesyl chloride were investigated. The synthesized photocatalysts were used for the photocatalytic decomposition of nitrous oxide. It was found out that the way of sulphur modification influences the degree of CN condensation and consequently its photocatalytic activity. The S-CN photocatalyst with the highest condensation degree proved to have the highest photocatalytic activity. Another important finding is connected with the type of nitrogen group on the surface of the photocatalyst analyzed by XPS. The NC2 group has a positive effect on the photocatalytic decomposition of nitrous oxide.

Acknowledgement
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P42

HOMOGENIZATION AND MIXING OF FLOW IN FLAT PANEL PHOTOBIOREACTOR

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In order to reach the industrial scale cultivation of microalgae biomass, it is necessary to optimize the operating conditions of existing cultivation systems and photobioreactors, which can currently mostly work effectively only on a laboratory scale. By changing the configuration of the inlet of the flat panel photobioreactor (FP PBR) chamber, it is possible to significantly influence the hydrodynamic conditions. However, by changing the inlet configuration, the high inhomogeneity of the flowing medium along the FP PBR chamber cannot be eliminated, which results in different residence times of the culture medium in the irradiated area. The aim of this work was to design a static mixer that could be installed in the FP PBR chamber. The static mixer should ensure the distribution of the medium flow throughout the cross-section of the chamber, ensure the homogenous residence time of the culture medium in the irradiated area, and further intensify the mixing of the culture medium. A numerical model was created for a detailed study of hydrodynamic conditions. The applicability of the numerical model was calibrated and validated based on the experimental tracer tracking method. Using a double bottom inlet configuration and an installed static mixer, the homogenization time was reduced by 17 % at a flow rate of 45 L min^{-1}, and by 34 % at a flow rate of 63 L min^{-1} in comparison to the empty FP PBR chamber. Using the created numerical model, it was also possible to study the distribution of the turbulent Reynolds number in the FP PBR chamber. Due to the homogeneous flow, the values of the turbulent Reynolds number in the cross-section of the chamber are also more evenly distributed. Elimination of dead zones in the FP PBR chamber can have a significant effect on the elimination of biofilm formation on the transparent walls of the FP PBR.

P43

OPERON STRUCTURE INFERENCE IN *CLOSTRIDIUM BEIJERINCKII* NRRL B-598 USING RNA-SEQ

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Current operon structure inference relies on utilization of online tools that provides predictions based on knowledge about intergenic distance of neighboring genes as well as the functional relationships of their protein products. This approach is not sufficient for accurate inference of operon structure as no information regarding co-expression of genes is taken into account. Moreover, such predictions are cumbersome in non-model organisms as relationships among their proteins are not known. Fortunately, the combination of wet lab data and data from web services using database searches can improve *in silico* inference of operon structure in individual bacterial or archaeal genomes a lot. Current research in biotechnology aims heavily on non-model organisms for their various phenotypic traits. An example can be found in the strain *Clostridium beijerinckii* NRRL B-598, a non-model butanol producer whose phenotype remains still to be explained on the molecular level. We used the complete genome sequence of the strain, available in the NCBI GenBank database under the accession no. CP011966.3, and predicted the operon structure for its 5,442 total genes using online tool Operon-mapper. Subsequently, we took 3,351 predicted operons and verified their co-expression using data from our previous transcriptomic studies. These include 36 samples of genome-wide transcriptomes of the strain under various conditions gathered using RNA-Seq technology. Finally, we were able to adjust predicted operons according to their co-expression.

P44

EFFECTS OF FURAN DERIVATIVES AND PHENOLIC COMPOUNDS ON ABE PRODUCTION BY *CLOSTRIDIUM BEIJERINCKII*

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Solventogenic clostridia can be used in solvent production via the acetone-butanol-ethanol pathway (ABE fermentation), while as a cheap and renewable waste substrate might serve lignocellulosic biomass. However, the production is negatively affected by the inhibitory compounds, which are formed during the pretreatment, in particular, furan derivatives and phenolic compounds are generated during acidic and alkali hydrolysis, respectively. The aim of this study was to determine the effects of furfural, 5-hydroxymethyl furfural, coumaric acid, and ferulic acid on the growth and production of ABE by two different strains of *Clostridium beijerinckii.* The minimum concentration negatively influencing growth and production was 3 g/L for furfural and 5-hydroxymethylfurfural, 1 g/L for ferulic acid, and 0.6 g/L for coumaric acid. Lower concentrations had an opposite stimulating effect, where production or both production and growth were improved comparing to the control experiment.

P45

METAL NANOPARTICLE SYNTHESIS MEDIATED BY *CANNABIS SATIVA* EXTRACT AND THEIR ANTIMICROBIAL ACTIVITY

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Metal nanoparticle antimicrobial activity has been a scientific “hot topic” in recent decades. Their emerging wide-spread application, however, poses new challenges regarding their production. The traditional methods of nanoparticle synthesis are energy-consuming and not very ecologically sustainable; the nanoparticle suspensions produced by chemical means may also contain toxic byproducts. In this study, we assessed the “green” production of silver nanoparticles using plant extract from hemp agriculture waste. These nanoparticles were characterized using UV-VIS spectrophotometry and TEM analysis. After that, the antimicrobial activity of biosynthesized nanoparticles was evaluated against planktonic cells of several strains of a gram-negative bacterium *Pseudomonas aeruginosa*. Subsequently, the bactericidal activity of these nanoparticles was explored by cultivating the suspension from planktonic cell experiment on a solid medium. The results show the biosynthesized silver nanoparticles exhibit measurable antimicrobial activity against *P. aeruginosa* cells.

P46

BIODIVERZITA PROKARYOT RADONOVÝCH PRAMENŮ V JÁCHYMOVĚ

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Bakterie a archea jsou všudypřítomné organismy, jejichž výskyt je omezen pouze extrémně nehostinnými podmínkami, jako je teplota (nad 121 °C), extrémně kyselé nebo alkalické pH (pod 0,5 a nad 12,5) a omezená dostupnosti vody [1]. Radonové prameny jsou příkladem extrémního prostředí, jejichž mikrobiom je však málo prozkoumán. Mikroorganismy v radonových pramenech jsou vystaveny působení několika abiotických faktorů zároveň, tedy přítomnosti ionizujícího záření a těžkých kovů, v některých případech i vysokých teplot. Radon je zdrojem alfa záření, které může způsobovat tvorbu reaktivních forem kyslíku a poškození biomakromolekul [2, 3]. Adaptace na stresové podmínky je podstatná pro přežití mikroorganismů v prostředí pramenů. Mezi hlavní mechanismy adaptace patří tvorba enzymatických a neenzymatických antioxidantů a účinná reparace poškozené DNA [4]. Radonové prameny v Jáchymově jsou jedinečné extrémně vysokým obsahem radonu [5]. V této práci byly z radonových pramenů v Jáchymově získány desítky bakteriálních izolátů. Taxonomická identifikace byla provedena pomocí metod MALDI-TOF a sekvenace 16S rRNA. Práce s izoláty byla zaměřena na studium bakteriálních kmenů odolných vůči působení ionizujícího UVC záření a oxidativního stresu (přítomnost volných radikálů v prostředí).

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P47

CULTIVATION STRATEGY AS A TOOL TO MITIGATE THE NEGATIVE EFFECT OF LIGNOCELLULOSE DERIVED INHIBITORS

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Lignocellulose biomass is the most abundant renewable feedstock available for various biotechnological production of bulk chemicals, such are ethanol, butanol, acetone, isopropanol, and others. The main bottleneck of its extensive utilization lies in its recalcitrance and as a consequence need for processing under harsh conditions which generate a broad range of inhibitors. To reduce the amount of inhibitors, a milder but less effective process might be applied or a detoxification step can be introduced. Both attitudes increase the cost of the process and question the ecological merit of the utilization of lignocellulose. Here, we introduce a cultivation strategy based on sequential feeding that enables full fermentation of toxic substrate, which inhibits the growth of production strain *Clostridium beijerinckii* when used in the batch mode. Comparable solvents yields (0.3 g/g) and butanol concentration (7.6 g/L) were obtained as with complex rich laboratory medium without inhibitors. Moreover, up to 75 % xylose was consumed together with nearly 50 % of acetic acid generated during alkali pre-treatment.

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ISOLATION OF FERULIC ACID FROM WHEAT BRAN USING VARIOUS ADSORBENTS

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Ferulic acid is a highly valued bioactive substance. It has a significant antioxidant effect, antimicrobial, anticancer, antiallergic, hepatoprotective, anti-inflammatory and antiviral effects. Due to these properties, the use of ferulic acid in the food, pharmacological and cosmetic industries is extensive. Recently, significant efforts have been made to find non-chemical processes for the preparation of this substance. One possible way to solve this issue is to valorize waste lignocellulosic materials i.e. from the cereal processing industry. According to FAOSTAT, the world's processing of wheat produces more than 120 million metric tons of bran which contain a significant amount of ferulic acid. In this work, four types of adsorbents (activated carbon, Amberlite XAD16, Amberlyst A21 and IRA-900Cl were tested for isolation purposes of ferulic acid from wheat bran treated with alkaline hydrolysis. The sorption and desorption efficiency of the materials used was verified in the study. Although the IRA-900Cl sorbent showed the highest adsorption efficiency, the sorbent Amberlite XAD16 was chosen for further experiments because, despite the lower adsorption efficiency, it showed the most effective desorption efficiency. The final yield of the optimized extraction process was 0,48 ± 0,02 g of ferulic acid from 1 kg of wheat bran.

P49

PRODUCTION AND ANALYSIS OF CRUDE BIOCHAR PRODUCED FROM WHEAT BRAN

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Biochar is solid material mainly produced by the pyrolysis of biomass. It is generally a carbonated material with high porosity and a high level of aromatization. Thanks to its properties, biochar is used in various industries, such as power production, agriculture, wastewater treatment, construction, pharmacy and many others. A significant advantage of biochar production is that it is often produced from agricultural and food waste, which corresponds to circular economics's philosophy. The physicochemical properties of biochar strongly depend on the feedstock type. An interesting raw material with potential for the production of biochar is wheat bran, a by-product of milling, which falls into lignocellulosic biomass. The main aspect of this work was developing a pyrolysis procedure and determining the products' physicochemical properties. The pyrolysis was performed in a furnace under an anaerobic nitrogen environment. Three pyrolysis temperatures were tested – 300, 400 and 500°C. Characterization of biochar was proceeded according to the European biochar certificate, which included size distribution analysis, SEM, BET surface area analysis, thermogravimetry (TGA), elemental analysis, FTIR spectral analysis and analysis of PAHs. FTIR, elemental analysis and SEM proved that 500 °C pyrolysis for 3 hours was optimal to produce well-carbonized biochar with the optimal structure. Yield of the process was 290,2 g of biochar from 1 kg of bran. Biochar contained a significant amount of K (45.7 ± 0.7 µg/g), and P (4.,8 ± 0.6 µg/g) and did not exceed the allowed limit of total PAHs (2.28 µg/g) set by European biochar certificate. The surface of the biochar significantly raised with the pyrolysis temperature with 3.4 m2/g for 500°C. This parameter can be substantially improved by subsequent chemical or physical activation. Wheat bran proved to be a material suitable as a feedstock for production of biochar with the potential for agricultural use.

P50

CIRCULAR BIODIESEL DOWNSTREAM SIDE-PRODUCTS UTILIZATION FOR UPSTREAM BIODIESEL VALORIZATION

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The first-generation biofuels production is primarily green waste-less process where side-streams are valorised, but not to their full extent and value. The post-fermentation corn oil side-product from bioethanol production is valorised as an oily feedstock in biodiesel facility. Corn oil processing influences process of biodiesel production, especially filterability and cold flow properties of final biodiesel due to its sterylglycosides and phytosterols content.

The side-product of biodiesel production is glycerol which might be utilized as a carbon source in liquid medium for growth of microbial producers.

The aim of this study is to evaluate glycerol utilization for biocatalysts production (sterylglycosidases) by recombinant producers *Escherichia coli* and *Pichia pastoris*. The closed loop of glycerol industrial application in biofuels processing is the key objective of the presented work, when used as a substrate for high added valuable enzymatic biocatalysts production (either in a whole-cell or enzyme form). The examined sterylglycosidase enzymes might be applied to remove existing technological and biodiesel´s quality problems in biorefineries caused by sterylglycosides and phytosterols presented in feedstock oil. The aim of presented work is to evaluate the sterylglycosides and phytosterols presence in corn oil during the biodiesel process flow and to find the appropriate point of production process where to apply recombinant biocatalysts to assure the most feasible process and high operational stability and improve its industrial applicability.

The further research is aimed to obtain representative and comparable data of bio-catalysis high specificity and activity.

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P51

EXPERIMENTAL ASSESSMENT OF CERAMZITE PARTICLE CHARACTERISTICS FOR DEM SIMULATION

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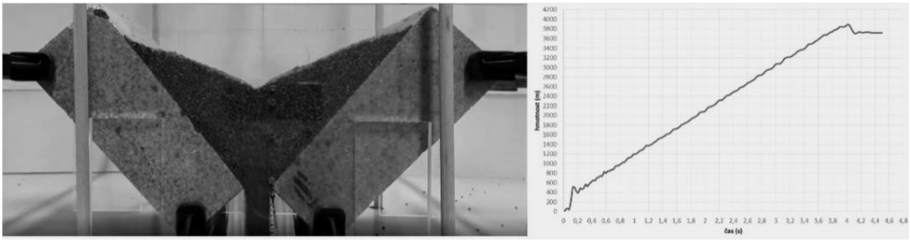
Preliminary results have been achieved in the description of transport phenomena in rotary kilns. Investigation of effect of construction inserts with different geometries and positions within the kiln on process parameters is objective of long-term research. Simulations focus particularly on particle motion and/or heat transfer. Commonly known methods such as DEM, DPM, DDPM are used in simulations.

The research is focused on the analysis and description of particles interactions in a rotating environment, namely a rotary kiln. So far, a model device was built and series of experiments were carried out to determine the physical parameters of the particles interaction models. The simple geometry of hopper was chosen to build up physical model. The front and rear walls are made from the plexiglass. Bottom walls are assembled from same bricks, those are used for the thermal insulation in the investigated kiln. Bricks are made from andalusite or fire clay. Ten inclination configurations (from 10 to 75 degrees from the horizontal plane) of the bottom hopper surfaces were investigated. The mass flow rate at the hopper discharge of expanded clay particles was recorded into a data file using weighing sensor and at the same time an audio-visual record of the level shape of bulk particles was performed.



Particles of ceramzite with size range 2-3 mm were used for measurement. The time trend of the collected mass of the particles for configuration of 50° is presented in the figure, together with the shape of the level of bulk particles in specific time of the experiment. The shape of the surface was observed, which will be described mathematically.

Identified parameters of the material interaction will be utilized for the numerical prediction of particles movement in the rotary kiln. It will be possible to use simulations for optimizing the internal construction and to better understand the processes in the rotary kiln for the production improvement of lightweight building aggregates.

P52

HOW DOES UNCERTAINTY OF THERMAL CONDUCTIVITY IMPACT MEASUREMENTS OF POOL BOILING HEAT TRANSFER COEFFICIENT?

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A typical measurement of pool boiling heat transfer coefficient is based on 1D conduction in a heated sample. Temperature of the boiling surface and heat flux are both calculated from temperature distribution inside the sample. Value of thermal conductivity of the sample is needed for calculation of heat flux and resulting heat transfer coefficient.

Researchers seldom measure thermal conductivity of their samples. A value, which corresponds to the material of the investigated sample, is typically adopted from the literature and treated as a constant. This approach is sometimes criticized as it might lead to significant errors of results.

This contribution quantifies the impact of thermal conductivity and its uncertainty on resulting heat transfer coefficients. Cases are discussed when careful assessment of thermal conductivity is required to reduce measurement uncertainty to an acceptable level.

P53

INVESTIGATION of MIXING TIME of SHEAR-THINNING FLUIDS

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This study deals with investigation of mixing time of shear-thinning fluids agitated by helical ribbon impellers by means of numerical methods. The mixing time was determined numerically by introducing tracer using species model in laminar régime. The effect of flow index on mixing time and pumping effect of the impeller were analyzed.

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THE INFLUENCE OF PROCESS PARAMETERS ON THE IMPREGNATION STAGE OF BEECH WOOD CHIPS

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The paper deals with the influence of process parameters on the CBC process impregnation step, which occurs during kraft cooking/delignification. The impregnated raw material was beech chips with 37 - 49% moisture content, which were sorted into the required fraction on a laboratory sorter in the first step. The impregnation tests focused on the water penetration content of the impregnation fluid into the beech chips due to its operational availability and physical properties, which are well known.

The gravimetric analysis determined the fluid content after the impregnation cycle as the ratio of the weight of the impregnated wood chip structure to that of dry wood. Impregnation tests over 24 hours were chosen to compare the maximum amount of fluid impregnated into the chip structure. The individual analyses show that the amount of fluid impregnated is greatly affected by the pressure used, while the temperature has a minor effect. This is illustrated by the results on the individual graphs. The highest content of impregnated liquid is recorded at a pressure of 5 bar, at a constant temperature, and the established time of the impregnation step. While maintaining constant conditions and increasing the pressure to 7 bar, a decreasing trend of the fluid impregnation content was observed.

Therefore, process parameters such as temperature and pressure significantly affect the impregnation step, which is a crucial part of the whole CBC process and significantly influences homogeneous delignification, overall yield, and the amount of rejects.

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VYUŽITÍ TECHNOLOGIE MSO K LIKVIDACI TETRACHLORETHYLENU

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Použití organických chlorovaných látek v moderní době stále narůstá a při jejich likvidaci konvenčními metodami je nutný náročný systém čištění spalin. Technologie Molten Salt Oxidation (MSO) je technologií, která využívá bezplamennou oxidaci pod hladinou taveniny soli. Při použití alkalických uhličitanů jsou kyselé odplyny zachyceny v tavenině, se kterou reagují za vzniku příslušných sloučenin a není tak potřeba složitý systém čištění spalin. Bylo provedeno pět experimentů na dvoureaktorové laboratorní aparatuře MSO. Jako alkalická tavenina byl v obou reaktorech použit čistý Na_2CO_3. Nastavená teplota na obou pecích byla 1050 °C. Experimenty se lišily dávkovaným množstvím C_2Cl_4 a rychlostí dávkování organického odpadu. Rychlost dávkování se odvíjela podle hodnoty účinnosti oxidace odpadu a byla v rozmezí od 2,5 ml/min do 5 ml/min. Průtok oxidačního vzduchu byl 4,5 l/min a byl veden do prvního reaktoru. Během experimentů byl měřen teplotní profil v každém reaktoru, byla prováděna analýza spalin a na konci experimentu byly odebrány vzorky taveniny, aby byl stanoven obsah vzniklých chloridů. Chloridy byly stanoveny argentometrickou titrací. Byla sledována účinnost oxidace C_2Cl_4 stanovením obsahu CO v odplynech. Hodnoty CO byly během experimentů značně vysoké: od 20000 ppm během prvního experimentu až po maximum 1200 ppm CO v posledním experimentu. Během experimentů se nám podařilo celý proces optimalizovat a tím zlepšit účinnost procesu. Vzniklý Cl_2 byl zachycen primárně v prvním reaktoru, kdy se účinnost záchytu pohybovala kolem 70 %. V druhém reaktoru byla účinnost záchytu velice nízká, pouze 0,7 %.

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GEOPOLYMERS: INFLUENCE OF ALKALINE ACTIVATOR CATIONS ON EFFLORESCENCE

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Geopolymer materials are widely studied due to their convenient properties. Owing to geopolymers, it is possible to process a large amount of industrial waste; from active fly ash, slag to inert waste which could be used as a filler. Geopolymers are highly heat-resistant, insoluble in water, can inhibit hazardous materials, and simultaneously achieve high strength. One of their disadvantages is efflorescence, which arises from the reaction of free alkali metal or alkaline earth cations with the surrounding environment. The efflorescence is not only unaesthetic but can also have a negative impact on the structure and properties of materials. Moreover, the formation of these salts influences the possibility of using geopolymer in common practice. Our aim is to thoroughly examine the effect of efflorescence on geopolymer materials.

Geopolymer materials were prepared by a standard procedure from the following raw materials. Aluminosilicate based on metakaolinite was used as the precursor and chamotte grit as a filler. Activators differ in the type of cations (Li^+, Na^+, K^+), and in the ratio of SiO_2/M_2O. The susceptibility to the formation of efflorescence was determined according to the standard ČSN EN 72 1565-13. Formed efflorescence was characterized by the XRD method to identify the mineralogical composition. Mechanical properties were measured, and the pore diameter was determined by mercury porosimetry.

The results showed an obvious impact of alkaline activator cations on the type of efflorescence. It was found that samples with lithium ions did not achieve as high compressive and flexural strengths as samples with sodium and potassium activators. Simultaneously, specimens with lithium cations had the largest pore radius. For this reason, it would be appropriate to further investigate the influence of lithium ions on geopolymer materials and to optimize these mixtures to prevent the formation of efflorescence and increase their mechanical resistance.

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SPOLUPRÁCE S AUSTIN DETONATOR, s.r.o.– OD VÝZKUMU PO TECHNOLOGII

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Společnost AUSTIN DETONATOR je tradičním výrobcem rozbušek pro průmyslové trhací práce a v České republice zahájila svou činnost v roce 1999 odkoupením výroby rozbušek z bývalé Zbrojovky Vsetín. Jednou z hlavních složek rozbušky je třaskavina, která se většinou, z hlediska bezpečnosti, vyrábí přímo v místě kompletace rozbušek. Historicky používané třaskaviny: fulminát rtuťnatý, azid olovnatý, pikraminan olovnatý, trinitrorezorcinát olovnatý a 1-(5-tetrazolyl)-3-guanyltetrazen hydrát (tetrazen), současným ekologickým požadavkům již neodpovídají. U prvních třech jmenovaných je problematický obsah těžkých kovů, u tetrazenu jeho nedostatečná stabilita. Většina používaných třaskavin obsahuje v těchto sloučeninách společný, a z hlediska REACH problematický, prvek olovo. Proto se již několik let usilovně pracuje na náhradách výše uvedených olovnatých sloučenin. Na vývoji této ekologicky přijatelné třaskaviny, bez obsahu olova, dlouhodobě spolupracuje s firmou Austin Detonator VŠCHT Praha. Počátek výzkumu je datován kolem roku 2010, kdy se začalo hovořit o náhradách azidu olovnatého a byl zahájen výběr vhodné „green“ třaskaviny. V letech 2012 až 2014 byly provedeny laboratorní testy možné přípravy této ekologické třaskaviny v malých množstvích, řádově do jednotek gramů. Postupně se zvyšovalo množství vyrobené látky, přešlo se z laboratorních nádob do čtvrtprovozní aparatury. Poté se začali řešit i problémy technologické, jako je výběr sušárny, znecitlivění produktu umožňující objemové dávkování a další nezbytné části technologického systému jako je např. chemické likvidace odpadních proudů. Na základě těchto výzkumů byla v letech 2015–2016 postavena poloprovozní jednotka na výrobu této třaskaviny, již kapacitně v řádech stovek gramů. V roce 2017 se začala vybírat lokalita k výstavbě budovy pro výrobu „green“ třaskaviny a byly zahájeny základní stavební práce. Paralelně s tím běželo vypracování „basic design“ této technologie. V letech 2018-2019 se zahájilo projektování a výroba technologických komponentů. V současné době je připraven projekt výrobní jednotky jako podklad pro stavební řízení. Dle plánů firmy Austin Detonator by nová výrobní jednotka mohla zahájit provoz v roce 2022.