51th

International Conference of the Slovak Society of Chemical Engineering

May 27 - 30

2025

PROCEEDINGS

Demänovská Dolina

Slovakia

#SSCHE2025

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SLOVAK
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Slovak Society of Chemical Engineering
Institute of Chemical and Environmental Engineering
Slovak University of Technology in Bratislava

PROCEEDINGS

51st International Conference of the Slovak Society of Chemical Engineering
SSCHE 2025

Hotel DRUŽBA

Jasná, Demänovská Dolina, Slovakia, May 27 - 30, 2025

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Proceedings of the 51^{st} International Conference of SSCHE
Jasná, Demänovská Dolina, May 27 - 30, 2025
© Slovak Society of Chemical Engineering, Bratislava, SK, 2025

ISBN: 978-80-8208-158-2
EAN: 9788082081582
Published by the Faculty of Chemical and Food Technology Slovak Technical University in Bratislava in Slovak Chemistry Library for the Institute of Chemical and Environmental Engineering; Radlinského 9, 812 37 Bratislava, 2024

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2	Anaerobic digestion as a solution for biowaste treatment in Slovakia (*Danielič, M., Variny, M.*)
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30	Microstructured PDMS surfaces for bacterial adhesion control (*Kříž, F., Nguyen, V., Tokárová, V.*)
31	Mini-tablets with Personalized Dissolution, Prepared by Fluid-Bed Granulation of Drug Nanosuspensions (*Mutylo, E., Navrátil, O., Waněk, A., Šembera, F., Štěpánek, F.*)
32	Modeling and Experimental study of LOHC systems based on toluene mixtures (*Tomasek, S., Egedy, A., Tóth, I., Lovas, L.*)
33	Modeling of Mass Transfer through an Ion-Exchange Membrane in Lithium Recovery by Donnan Dialysis (*Tomášik, M., Markoš, J., Červeňanský, I., Hlavatý, L.*)
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54 There is something in the air: an overview of allicin-based antibacterial materials (*Mašková, L., Lizoňová, D., Zelenka, P., Tokárová, V., Kašpar, O.*)

55 Thermochemical conversion modelling of multilayer packaging waste using Aspen Plus (*Khurram, A., Escudero Sanz, F., Carrier, M., Haydary, J.*)

56 Valorization of Charry Pit Waste: Efficient Oil Extraction for Biodiesel Production (*Knežević-Jugović, Z., Jakovetić Tanasković, S., Šekuljica, N., Boroš, K., Manou, D., Skoufi, M., Dajić Stevanović, Z.*)

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08:00–09:30 GRAND A1, Plenary lectures

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08:45 Replacement of trichloroethylene in the extraction of crude caprolactam (*Obalová, L., Leštinský, P., Maršolek, P., Vaštyl, J., Koumar, J., Korpas, J., Maxa, M.*)

09:30 Coffee break

10:00–12:40	**GRAND A1, Lectures: Separation processes and transport phenomena**
10:00	Enzyme synthesis and continuous flow separation of (R)-1-phenylethanol in a modular microfluidic system (*Sauer, L., Přibyl, M.*)
10:20	Green analytical strategies for selenium determination using chromatographic and spectrometric methods (*Mot, A., Covaci, E., Boşca, B., Dudu, A., Frentiu, T.*)
10:40	Intensification of Separation Processes in a Model Electrodialysis Unit (*Pagáč, J., Slouka, Z., Láznička, V., Tichý, D.*)
11:00	Ion concentration polarization for separation of charged species (*Slouka, Z., Tichý, D., Škrhák, M.*)
11:20	Mathematical modeling of an ion transfer in a donnan dialysis process via nernst-planck equation (*Hlavatý, L., Sedlák, L., Komačková, E., Červeňanský, I., Markoš, J.*)
11:40	Reaction transport phenomena at ion-exchange membranes in DC electric field (*Láznička, V., Slouka, Z.*)
12:00	Removal of organic acids from fermentation broth by pertraction hollow fiber membrane module (*Mihaľ, M., Červeňanský, I., Markoš, J.*)
12:20	Use of multifiber membrane module for lithium recovery (*Sedlák, L., Komačková, E., Droščínová, L., Fehér, J., Hlavatý, L., Markoš, J., Červeňanský, I.*)

08:50–12:10	**GRAND B2, Prednášky: Riešenia pre energetickú transformáciu priemyslu (SK industry section)**
08:50	**Otvorenie priemyselnej sekcie**
09:00	Aktuálne otázky plynárenstva na Slovensku (*Kvasňovský, R.*)
09:15	Nový stavebný zákon (*Sadloňová, M.*)
09:35	**Coffee break**
10:10	Čo je to energetická transformácia priemyslu? (*Buchan, V.*)
10:30	Tepelné čerpadlá: Dekarbonizácia a efektívne využitie odpadového tepla (*Jurovich, M.*)

10:50	Elektrifikace procesního tepla: Cesta k bezemisnímu průmyslu (*Tesař, F.*)
11:10	Dekarbonizácia prepravy vďaka riešeniam s pridanou hodnotou (*Kamenský, R.*)
11:30	Linda - Vývoj a implementácie elektronických prevádzkových záznamov pre vybrané energetické prevádzky v závode Volkswagen Slovakia (*Chávez Fuentes, J.*)
11:50	Monitoring priebehu krátkodobého prietoku oleja hydraulického lisu v oceliarenskom priemysle pomocou ultrazvukového monitora prietoku (*Iľko, J., Mudrá, M.*)
12:00–14:00	**Lunch**

14:00–17:00 GRAND A1, Lectures: Bioprocess and biotechnology

14:00	Biocompatibility of ionic liquids and their recovery from aqueous solutions (*Schlosser, Š., Krištofíková, Ľ., Marták, J., Annus, J., Polakovič, M.*)
14:20	Development and optimization of chromatographic methods for the separation of recombinant tau proteins (*Kotuličová, S., Molnár, T., Majerová, P., Kováč, A., Polakovič, M.*)
14:40	Enzymatic hydrolysis efficiency of different industrial hemp biomass fractions: A comparative study of two cultivars (*Karpiński, G., Dąbkowska-Susfał, K., Januszewski, J., Pilarek, M., Krzysztoforski, J.*)
15:00	Impact of substrates and deep eutectic solvents on thermal stability and biocatalytic properties of beta-galactosidase during transglycosylation (*Koššuthová, A., Antošová, M., Bauerová-Hlinková, V., Bauer, J., Polakovič, M.*)
15:20	Intensified Sustainable Approaches for Separation of Glutaric Acid (*Thakre, A., Shende, D., Wasewar, K.*)
15:40	Silica-based aerogels as functional materials supporting transgenic root proliferation and bioactive metabolite production (*Wierzchowski, K., Nowak, B., Kawka, M., Bober, S., Sykłowska-Baranek, K., Pilarek, M.*)
16:00	**Coffee break**
16:20	Sustainable Separation of Bio-Carboxylic Acids using Deep Eutectic Solvents (*Thakre, A., Shende, D., Wasewar, K.*)
16:40	Biochemical processes of lignocellulosic biomass conversion (*Ledakowicz, S.*)

17:00–18:20	**GRAND A1, Lectures: Energy transition and circular economy**
17:00	Hydrogen Position in the Energy Transition: Analysing the Competitiveness of Low-Emission Technologies (*Polakovičová, D., Variny, M.*)
17:20	Implementation of desalination technology in ammonium thiosulfate manufacturing (*Turinič, N., Variny, M., Buchan, V.*)
17:40	Modelling metal deposition on a 3D electrode in a hybrid flow battery: Validation by microcomputed tomography imaging (*Blahušek, V., Gráf, D., Staś, J., Bureš, M., Zubov, A., Mazúr, P.*)
18:00	Comparison between Ni/ZSM-5 and NiMo/AlO Catalysts in the Hydrocracking of FischerTropsch Wax Reflected in the Properties of Middle Distillates (*Horváth, D., Tomasek, S.*)

14:00–17:20	**GRAND B2, CVaV workshop: Priemyselné emisie a ESG: Riešenia z praxe (SK industry workshop)**

16:00–16:20 **Coffee break**

19:00–03:00 **Conference party**

Thursday

08:40–11:40	**GRAND A1, Lectures: Pharmaceutical engineering and processes**
08:40	An Introduction to the Stochastic Nature of Nucleation in Freeze-Drying (*Filčáková, A., Krošláková, S., Annus, J., Rajniak, P.*)
09:00	Computational insight to observed collective phenomena of lipid membrane permeation (*Císařová, T., Lněnička, J., Balouch, M., Štěpánek, F., Berka, K.*)
09:20	Development of advanced methodology for in vitro testing of long-acting injectable depot systems (*Nagy, O., Balouch, M., Štěpánek, F.*)
09:40	Drug permeability: commonly misinterpreted bioavailability governing factor (*Balouch, M., Storchmannová, K., Berka, K., Štěpánek, F.*)

10:00 Coffee break

10:20 Encapsulation in Liposomes and the Critical Role of the Encapsulated Substance (*Roudný, M., Balouch, M., Hanuš, J., Štěpánek, F.*)

10:40 Experimental and theoretical investigation of spray drying: What can happen in single droplets (*Rajniak, P.*)

11:00 Multi-physics problems in particulate engineering 3 case studies (*Sinka, C.*)

11:20 Development and Optimization of a Continuous Liquid Antisolvent Precipitation Device for Nanocrystalline Formulations (*Hládek, F., Nagy, O., Smrcka, D., Štěpánek, F.*)

11:40–12:00 GRAND A1, Lecture: Process design and process intensification

11:40 Production of carboxylic acids from organic waste via electro-fermentation: selectivity, recovery and electrochemical upgrading opportunities (*Koók, L., Rózsenberszki, T., Kovács, S., Kucsera, K.*)

09:00–11:20 GRAND B2, Emerson workshop: Emerson industrial innovations (SK industry workshop)

12:00–14:00 Lunch

14:00–16:40 GRAND A1, Lectures: Environmental chemical engineering

14:00 Evaluation of the influence of additives in model mixtures on the quality of pyrolysis products (*Klemencova, K., Grycová, B., Strakosova, J., Lestinsky, P.*)

14:20 Exegesis of Potential of Ionic Liquid for Absorption of Carbon dioxide (*Athankar, K.*)

14:40 Ex-situ tar elimination during densified refuse-derived fuel (d-RDF) gasification (*Nazari, M., Koritár, M., Haydary, J.*)

15:00 Magnesium Recovery from Brine via Reactive Membrane Crystallization Using Hollow-Fiber Modules (*Komačková, E., Sedlák, L., Hlavatý, L., Červeňanský, I., Markoš, J.*)

15:20 Optimization of thermochemical conversion feedstock parameters for an integrated waste (bio)refinery (*Koritár, M., Nazari, M., Haydary, J.*)

15:40 **Coffee break**

16:00 Reuse of quaternary treated wastewater for agricultural irrigation, reality or fantasy? (*Juríк, J., Zakhar, R., Takács, F., Bodík, I., Kalina, A., Rácik, M.*)

16:20 Start your research with LRI ENREGAT! (*Grycová, B., Obalová, L.*)

16:40–17:40 **GRAND A1, Lectures: Digitalization and process control**

16:40 Chemical process response analysis to single and multiple input parameter deviations. (*Myšiak, J., Labovský, J., Jelemenský, Ľ.*)

17:00 Reinforcement learning for chemical process control (*Szatmári, K., Németh, S., Kummer, A.*)

17:20 Why we waste the time of educated people on trivial activities - how to know more by doing less (*Krzyzostaniak, M.*)

17:40 **Closing of the conference**

18:00–20:00 **Dinner**

Friday

08:00–12:00 **Departure of participants**

Plenary lectures

A NEW ERA IN OLEFIN METATHESIS: CATALYSIS TOWARDS A SUSTAINABLE FUTURE

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Growing concerns surrounding plastic waste management necessitate the development of diverse strategies and technologies to support the transition toward sustainable, circular materials. One particularly promising approach to addressing the persistent challenge of fossil-based plastic waste - such as polyethylene - is the design of innovative catalytic processes that upcycle waste into more sustainable, value-added products. Among these, olefin metathesis catalytic systems have emerged as powerful tools for transforming durable polyethylene waste into valuable chemical intermediates, which can be further utilized to produce high-value materials, including chemically recyclable and biodegradable plastics.

This work focuses on the development and application of N-alkyl-substituted Cyclic(Alkyl)(Amino)Carbene (CAAC)-Ru catalysts with "inverted" chemical structures, as well as bicyclic (Alkyl)(Amino)Carbene (BICAAC)-Ru complexes, both of which demonstrate enhanced activity in isomerization metathesis (ISOMET) reactions. These catalysts are used in tandem with a ruthenium-based double bond isomerization co-catalyst, $(RuHCl)(CO)(PPh_3)_3$. The process begins with the slow pyrolysis of post-consumer polyolefin waste, generating pyrolysis oils enriched in olefins. In the subsequent ISOMET step, the tailored olefin metathesis catalysts are combined with the isomerization catalyst to selectively convert these olefins into propylene.

The resulting olefin metathesis/isomerization catalyst systems show remarkable efficiency in converting post-consumer plastic waste into propylene. Notably, successful scale-up to a 900 mL reactor system and repeated batch testing confirmed the long-term operational stability of the catalyst system.

The metathesis of sterically crowded alkenes remains a significant challenge due to reduced catalyst accessibility and reactivity at the hindered double bonds. These substrates often exhibit sluggish reaction rates, poor conversions, or lead to catalyst deactivation. Overcoming this limitation requires the development of more robust and selective catalyst systems capable of tolerating steric bulk while maintaining high activity and functional group compatibility. Advances in ligand design - especially the development of novel bicyclic(alkyl)(amino)carbene (BICAAC)-based catalysts - offer promising solutions to the challenge of metathesis involving branched polymers, paving the way for broader applications in polymer chemical recycling. This talk will highlight recent progress and remaining challenges in olefin metathesis-based approaches to polymer recycling.

Replacement of trichloroethylene in the extraction of crude caprolactam

Lucie Obalová[1], Pavel Leštinský[1], Petr Maršolek[1], Jana Vaštyl[1], Jiří Koumar[2], Jakub Korpas[1],
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Key words: Caprolactam; Extraction; Mixed solvent; Trichlorethylene; Karr column

Caprolactam is the precursor to Nylon 6, a widely used synthetic polymer. Most of the world's caprolactam production involves its synthesis from cyclohexanone via the Beckmann rearrangement. The purity requirements for caprolactam are stringent, as even trace amounts of impurities can significantly affect the physical and mechanical properties of Nylon 6. Due to the presence of both polar and nonpolar impurities in crude caprolactam, purification traditionally includes forward extraction with a nonpolar solvent such as trichloroethylene, followed by back-extraction with water and multistage distillation.

This study focuses on the search for safer, non-carcinogenic alternatives to trichloroethylene in caprolactam extraction. Since a high distribution coefficient of caprolactam in the forward extraction process is undesirable for subsequent back-extraction with water, the alternative solvent should exhibit a distribution coefficient for caprolactam similar to that of trichloroethylene. Additionally, low mutual solubility with water, favorable physical properties, a low distribution coefficient for impurities, and acceptable cost are further requirements.

Suitable solvents were estimated using Hansen solubility parameters. Experimental liquid-liquid equilibrium data, along with key physical properties affecting mass transfer (density, viscosity, and interfacial tension), were determined for the design of Karr extraction columns with reciprocating plates, as used in caprolactam refining. The model was further validated through performance trials with an actual extraction unit employing trichloroethylene in caprolactam refining.

Acknowledgement

This work was financially supported by the project "Continuous caprolactam refining" (No. TRIO FV40040.) Experimental results were accomplished by using Large Research Infrastructure ENREGAT supported by the Ministry of Education, Youth and Sports of the Czech Republic under project No. LM2018098.

Separation of enantiomers by membrane processes

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Abstract

Membrane technologies provide optimal conditions for controlling enantiomer synthesis and purification in continuous production, offering significant advantages over batch manufacturing. One of the key drivers for developing such technologies is the growing demand for enantiomerically pure pharmaceutical drugs, as enantiomers can exhibit opposite therapeutic effects or varying levels of efficacy and side effects. However, despite advancements in asymmetric synthesis and separation techniques, achieving high-purity enantiomers remains a considerable challenge.

This plenary lecture reviews the progress made in membrane-based chiral separation over the past two decades. In addition to describing and critically evaluating the current state of the field, we highlight the advantages and unique characteristics of membranes in enabling the production of enantiomerically pure compounds.

While sorption played a crucial role in pertraction, significantly enhancing the separation of racemic mixtures, pressure-driven membrane processes enabled continuous and accelerated operation [1]. This capability demonstrates the potential for large-scale, continuous production of enantiopure compounds, paving the way for new commercial applications and addressing the increasing need for efficient chiral separation techniques. A detailed comparison with previously reported chiral membranes [2,3] will be discussed at the conclusion of the plenary lecture.

Acknowledgement: This research was funded by the Czech Science Foundation, 23-06152S.

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

Lectures

Lectures: Bioprocess and biotechnology

Biochemical processes of lignocellulosic biomass conversion

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Key words: biomass pretreatment techniques, anaerobic digestion, syngas fermentation, bioethanol, biohydrogen, bioelectrochemical processes

In the face of a changing energy economy based on fossil fuels, we need to move towards renewable energy sources. And one such resource that meets these criteria is biomass. It is well known that in addition to thermochemical processes, biochemical methods of lignocellulosic biomass (LCB) processing play an important role in the production of renewable fuels and value-added products. Biochemical conversion involves the use of enzymes and microorganisms as catalysts in the breakdown of biomass into biofuels. The main biochemical conversion routes are anaerobic digestion (AD), fermentation, photobiological hydrogen production and bioelectrochemical processes that take place in microbial electrolysis cells (MEC). The biochemical route has a long cycle time and is less efficient at breaking down recalcitrant biomass materials. For this reason, a combination of thermochemical and biochemical routes may be promising, taking advantage of both methods for the processing of biofuels. But due to limited space this review is limited to the biochemical processes involved in biorefinery. After a brief characterization of lignocellulosic biomass (LCB) and the pretreatment techniques used to disrupt lignin structure, depolymerize cellulose, this review considers four main pathways for LCB biochemical conversion: Digestion (anaerobic); Fermentation (syngas, ethanol, butanol and dark fermentation); Photobiological hydrogen production; Bioelectrochemical processes in MEC. The integration of thermochemical processes with biological conversion of LCBs is an opportunity for further biorefinery development. Conclusions and future perspectives for the integration of biological and thermochemical LCB conversion processes are highlighted.

Acknowledgment: *Financial support from the National Science Centre (Poland) under project number 2021/43/B/ST8/00298 is acknowledged.*

Biocompatibility of ionic liquids and their recovery from aqueous solutions

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Keywords: biocompatibility, phosphonium ionic liquids, adsorption, recovery

Transformation of fuel and chemical industry based on fossil raw materials to biorefineries based on renewable biomaterials require development of new approaches in products separation or in biomass pretreatment processes. Solvent extraction may have important role in biorefineries what will require development of novel solvents. Ionic liquids (ILs) could be candidate as nonvolatile effective solvent. Their biocompatibility is an important parameter for their successful application in bioprocesses. Organic acids are important platform chemicals for production of wide variety of organic chemicals and fuels. They can be effectively extracted with phosphonium ionic liquids but not adequate care was paid to their biocompatibility with microbial acid producents what is addressed in this work.

Results of biocompatibility tests of newly developed ILs [1] with bacterial producent of lactic acid *Bacillus coagulans* (*B. coagulans*) will be presented. The most commercially available hydrophobic phosphonium and ammonium ILs are more or less toxic to *B. coagulans* what is connected probably with their not enough low solubility in water. Influence of cation and anion structure on IL biocompatibility was studied. New ILs based on trioctyldodecylphosphonium cation and branched carboxylate anions are compatible with *B. coagulans* and are liquid at room temperature [1]. ILs with n-decanoate anion are good solvents when diluted with dodecane but pure IL is solid what could be technological problem, thus application of branched carboxylate anions could be solution.

Hydrophobic ILs are more expensive comparing to molecular solvents and it is important recover them from diluted process aqueous solutions what is important also from environmental point of view. It was found that hydrophobic phosphonium ILs can be effectively adsorbed by neutral polymeric adsorbent from aqueous solutions saturated with ILs. Capacity of packed column for decontamination of model water saturated with phosphonium IL was more than 298 BV (bed volumes) while full column capacity of continuous work was not achieved after 40 hours of operation.

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Development and optimization of chromatographic methods for the separation of recombinant tau proteins

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Key words: Tau proteins, separation, size-exclusion chromatography, hydrophobic interaction chromatography

In neurons, tau proteins play key role in the stability of microtubules and in the efficiency of axonal transport through regulated interactions with tubulins, which are affected by isoform variations and phosphorylation. However, pathological modifications, specifically hyperphosphorylation, lead to microtubule disruption and to the formation of tau aggregates, including oligomers and neurofibrillary tangles. These aggregates negatively impact neuronal function and contribute to neurodegenerative diseases. The intercellular transfer of these aberrant tau proteins induces neuronal cell death and the advancement of neurodegenerative diseases, particularly in Alzheimer's disease.

The objective of this study was to design an effective chromatographic process for the separation of tau protein isoforms. The inherent similarity in primary structure among these isoforms complicates separation due to their comparable physicochemical characteristics. The potential of size-exclusion chromatography, which enables separation within a narrow size range, was explored. Additionally, hydrophobic interaction chromatography was investigated to leverage differences in hydrophobicity among isoforms.

To enhance separation efficiency, size-exclusion chromatography columns with varying pore sizes, connected in series with increasing pore diameter, were tested. Buffers of higher ionic strength were employed to eliminate non-specific interactions. Some isoforms, despite their minor molecular weight differences, were successfully separated using a 0.01M Tris buffer (pH 7) supplemented with 0.5M NaCl and GuHCl as mobile phase.

Initial experiments using hydrophobic interaction chromatography were conducted with a reversed-phase column and a 5-80% acetonitrile gradient in 0.1% formic acid as mobile phase. Preliminary chromatograms showed visible peaks, suggesting potential separation of tau protein isoforms.

Acknowledgements
This work was supported by grant from the Slovak Research and Development Agency (Grant number: APVV-21-0321).

Enzymatic hydrolysis efficiency of different industrial hemp biomass fractions: A comparative study of two cultivars

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Key words: lignocellulosic biomass, biorefineries, renewable feedstock, stems, leaves, Santhica, Futura

Industrial hemp is a promising, renewable feedstock for biorefineries. Low agricultural needs, and considerable biomass yield from a hectare of the plantation every season make industrial hemp an interesting raw material for renewable feedstock utilization studies. Particularly hemp fibers, being a lignocellulosic biomass, may be enzymatically broken down to monosaccharides. These hydrolysates, rich in glucose and xylose, after appropriate supplementation can serve as a culture medium for microorganisms able to produce useful chemical compounds. In this study, an enzymatic hydrolysis of two cultivars of the industrial hemp, Santhica and Futura, was conducted on three separate fractions of these plants: stems, leaves and spent flowers. The flowers were previously extracted with supercritical carbon dioxide to obtain pharmaceutically useful compounds e.g. cannabinoids, terpenes etc. The aim of this study was to compare the enzymatic saccharification efficiency of different waste hemp fractions. Enzymatic hydrolysis was preceded by chemical pretreatment of dry hemp material. First the stems were milled, leaves and flowers were crushed. Then all the fractions were treated with sodium hydroxide solution for 20 minutes at 121°C, 0,1 MPa. After the hot stage, the treated hemp fractions were washed with distilled water and dried in room temperature before hydrolysis. The hydrolysis took 72 h in citrate buffer at 50°C and pH=5 with sodium azide as an antimicrobial agent, sampled twice a day and the monosaccharides concentration was measured using HPLC method. The initial biomass loading was 60 g/dm^3 and the enzyme concentration (Cellic CTec2, SigmaAldrich) was 9% (w/w). The obtained results exhibit a strong advantage of hemp stems over other fractions, due to the higher content of hydrolysable polysaccharides, with final glucose concentration after 72 h of hydrolysis reaching >30 g/dm^3. Glucans hydrolysis efficiency reached 74,33±1,15% for Santhica and 79,68±2,10% for Futura, and for xylans' efficiency reached 82,39±2,10% and 95,73±6,17% for Santhica and Futura, respectively. Efficiency of the hydrolysis never reached over 20% for both glucans and xylans in the leaves, furthermore the saccharides concentration increased for the first 24 h and then started to decrease to reach zero after 72 hours.

Impact of substrates and deep eutectic solvents on thermal stability and biocatalytic properties of beta-galactosidase during transglycosylation

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Key words: β-galactosidase, transglycosylation, deep eutectic solvents, stability, activity

Aspergillus oryzae β-galactosidase is a glycosyl hydrolase with transglycosylation activity, enabling glycosylation of bioactive compounds such as tyrosol, a phenylethanoid with known antioxidant properties. This study explores how substrates and deep eutectic solvents (DESs) affect enzyme stability and activity during the synthesis of tyrosol β-D-galactoside (TG).

Enzyme stability was assessed using both nano differential scanning fluorimetry (nanoDSF) and circular dichroism (CD) spectroscopy to provide complementary structural and thermal insights. NanoDSF revealed that lactose stabilized the enzyme in a concentration-dependent manner, increasing the melting temperature (Tm) from 69.5°C (in buffer) to 76.5°C at 0.83 M. To correlate these thermal transitions with structural changes, CD spectra were recorded at 42°C, 60°C, and 70°C. At 42°C, β-galactosidase retained its native secondary structure. Minor changes were observed at 60°C, while spectra at 70°C indicated partial unfolding, primarily involving helical structures, without complete denaturation confirming and complementing the nanoDSF data.

Among DESs tested, betaine-based solvents provided the greatest stabilizing effects. However, several DESs altered enzyme specificity, often favoring hydrolysis over transglycosylation. Polyols present in DESs could act as alternative glycosyl acceptors, impacting product profiles. Both glycerol and tyrosol inhibited enzyme activity and TG synthesis, though glycerol also enhanced thermal stability.

While CD spectroscopy could not assess structural changes in the presence of substrates or DESs due to signal interference, the combined data from CD and nanoDSF offer a comprehensive view of the enzyme's conformational behavior under different conditions. These findings highlight the importance of reaction environment in tuning β-galactosidase performance for sustainable synthesis of glycosylated bioactives.

Acknowledgment: This work was supported by grants from the Slovak Research and Development Agency (Grant number: APVV-20-0312) and the Scientific Grant Agency of the Slovak Republic (Grant number: VEGA 1/0515/22).

Intensified Sustainable Approaches for Separation of Glutaric Acid

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Key words: Intensification, Sustainable, Glutaric Acid, Reactive extraction, Ionic liquids, Deep Eutectic Solvents, Ultrasound Assisted, Microwave Assisted

Glutaric acid is a five-carbon dicarboxylic acid with the chemical formula C5H8O4, obtained from fermentation is known for its diverse applications in various industries, including pharmaceuticals, plastics, and food additives. The separation of glutaric acid form the fermentation broth using green solvents is crucial for both process efficiency and product purity. The sustainable separation of glutaric acid from aqueous solutions is a vital process in the production of bio-based chemicals, playing a crucial role in promoting green chemistry and minimizing environmental impact. Conventional approaches are limited with many drwabacks including toxicity and negative nevrionment impact, high energy requirment and capital cost. Further, process intensification can contribute significantly in development of sustianble process for the separation of glutaric acid. The various intensified sustianble approaches comprises: reactive extraction, natural solvents, ionic liquids, deep eutectic solvents, mucrowave assisted, ultrasound assisted, hybrid and combination of solvents, microfulidic separation, inverted colied separation etc. Theoretical aspects of these processes have been discussed based on key features. Also few experimental results on separation of glutaric acid using natural non-toxic solvents, physical extraction, reactive extraction, ionic liquids, deep eutectic solvents, mucrowave assisted, ultrasound assisted, hybrid and combination of solvents, etc. have been presented. Key factors impacting separation efficiency, including solvent composition, molar ratios, hydrogen bonding interactions, and operational conditions, are thoroughly examined. The study underscores the effectiveness of various solvent and approaches in extracting biochemicals like carboxylic acids, amino acids, and natural phenolic compounds, achieving enhanced selectivity and yield compared to traditional methods. The presented innovative technique has demonstrated significant potential to separation practices. Additionally, the reusability and stability of solvents under diverse operational conditions reinforce their economic and ecological advantages. These advancements align with global efforts toward greener and more efficient bioprocessing technologies.The obtained results are usful for the selction of suitable intensified sustianble approach and its design for a specific application. This work establishes a scalable, green approach for glutaric acid recovery, advancing the sustainable production of valuable bio-based acids from fermentation and supporting broader applications in green separation technologies.

Silica-based aerogels as functional materials supporting transgenic root proliferation and bioactive metabolite production

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Keywords: silica-based aerogels, transgenic roots, secondary metabolites, plant biomass, bioprocess intensification, metabolism induction

Plant, using their secondary metabolism pathways, produce a wide range of bioactive compounds that can be utilized by the pharmaceutical industry. Many plant-derived molecules exhibit anticancer activity, which makes them interesting candidates for cancer treatment drugs. Transfer of plant biomass to a culture system with strictly controlled parameters (in vitro system) allows for the optimization of the process of secondary metabolites biosynthesis and makes plant-derived molecule production independent from environmental variability or geographical, ecological, or political constraints. In vitro conditions provide the unique ability to modify culture systems by implementation of bioengineering techniques aimed at intensifying the production of desired secondary metabolites. Actually, the most effective bioengineering techniques for enhanced secondary metabolite production are: elicitation (induction of secondary metabolism pathways by biotic or abiotic agents), immobilization of biomass (its spatial confinement by means of inert media), and in situ product removal techniques (reception of products into an additional phase of the culture system limiting negative feedback of secondary metabolism pathways). Furthermore, the specificity of the plant biomass in vitro culture also makes it possible to scale up the bioprocess effectively using bioreactors.

The aim of the study was to develop a novel aerogel-based *in vitro* system for the enhanced biosynthesis of secondary metabolites. The influence of (i) aerogel form, (ii) the pore size in aerogel, (iii) the aerogel functionalization, and (iv) chitosan concentration in hybrid silica-chitosan aerogel on the *Rindera graeca* transgenic root biomass proliferation and secondary metabolite (i.e., naphthoquinone) production have been determined.

The highest yield of naphthoquinone production has been observed for transgenic root cultures using hybrid silica-chitosan aerogel containing $40\%_{m/m}$ of chitosan. In the case of plant biomass proliferation, the highest value of fresh biomass increase has been noticed for transgenic root cultures using silica aerogel with methyl groups.

Acknowledgments

This work has been funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program (YOUNG PW II).

Sustainable Separation of Bio-Carboxylic Acids using Deep Eutectic Solvents

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Key words: Sustainable Separation, Bio-carboxylic Acid, Deep Eutectic Solvents, Extraction Efficiency, Parameters, Design

Biocarboxylic acids are crucial platform chemicals derived from the biological conversion of renewable resources. Separating carboxylic acids from fermentation broth is significant and challenging. Biocarboxylic acids can be extracted from fermentation broths using reactive liquid-liquid extraction, which has been extensively researched. However, the commonly used petroleum-based solvents should be replaced with greener alternatives. Deep eutectic solvents have become a highly potential type of green solvent, with a wide array of well-documented applications. DESs, an ionic liquid, are created by mixing a hydrogen bond acceptor (HBA), like a quaternary ammonium salt, with a hydrogen bond donor (HBD), such as a metal halide. These solvents possess unique physicochemical properties such as non-toxicity, renewability, biodegradability, and ease of preparation, making them attractive green solvents. Rising concerns about environmental sustainability have driven many industries to replace synthetic organic solvents with greener alternatives in their manufacturing processes. Given the importance of DES as a solvent, the present paper focuses on an exhaustive literature study on DES application for the separation of carboxylic acid. Further, various types of DES used for carboxylic acid separation along with the effect of various parameters on performance efficiency have been discussed.

Lectures: Environmental chemical engineering

Evaluation of the influence of additives in model mixtures on the quality of pyrolysis products

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Keywords: Pyrolysis, plastics, catalyst, additives

With the growing world population and the increasing demands on living conditions, plastic production is also increasing, and plastic waste is becoming an increasingly pressing problem. Plastic waste contains various types of additives that can be released into the environment and negatively affect it. Additives are added to plastics to improve their properties; on the other hand, additives can affect chemical reactions and the quality of recycled products. In this study, the effect of naturally occurring additives on the chemical recycling of polyolefin model mixtures with additives was investigated. The additives facilitated the cracking of long polymer chains, which led to higher yields of light hydrocarbons during thermo-catalytic pyrolysis compared to fresh polymer. However, the additives generally reduced the formation of aromatic nuclei during thermo-catalytic pyrolysis, with carbon black being an exception, as they promoted the development of aromatics and increased the formation of xylene and toluene during thermo-catalytic pyrolysis. The type of additive in waste plastics significantly influenced both the yield and quality of the pyrolysis products. An appropriate combination of additives results in increased formation of aromatic hydrocarbons.

Acknowledgments

Experimental results were accomplished using REFRESH – Research Excellence For Region Sustainability and High-tech Industries, CZ.10.03.01/00/22_003/0000048 and Large Research Infrastructure - Energy Waste Recovery and Gas Treatment supported by the Ministry of Education, Youth and Sports of the Czech Republic under Project Number LM2023056.

Exegesis of Potential of Ionic Liquid for Absorption of Carbon dioxide

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The atmospheric concentration of industrial gases, especially CO_2, has been persistently rising, reaching 424 ppm by November 2024, which correlates with an increase in global temperatures. In view of this, CO_2 mitigation technologies must be developed. As of now, absorption of CO_2 using amines is the most prevalent technology for CO_2 capture from post-combustion flue gas. However, this process requires high energy for solvent regeneration. Therefore, researchers have suggested ways to get around the drawbacks of amine process. Ionic liquids, characterized as salts with melting points below 100°C, have garnered interest in recent years as potential solvents for CO_2 absorption, owing to their low vapor pressures, high thermal stability, and significant CO_2 uptake capacity. This review articulates the molecular mechanisms underlying CO_2 capture with ionic liquids. It explores the properties of ionic liquids, the characterization of CO_2-ionic liquid systems, and the effects of operating conditions on the CO_2 uptake capacity of ionic liquids. It underscores the role of cations, anions, and functional groups in determining the solubility of CO_2 in ionic liquids, as well as their biodegradability and toxicity.

Keywords: Absorption, CO_2 capture, ionic liquids, global warming, solvent regeneration.

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Ex situ tar elimination during densified refuse-derived fuel (d-RDF) gasification.

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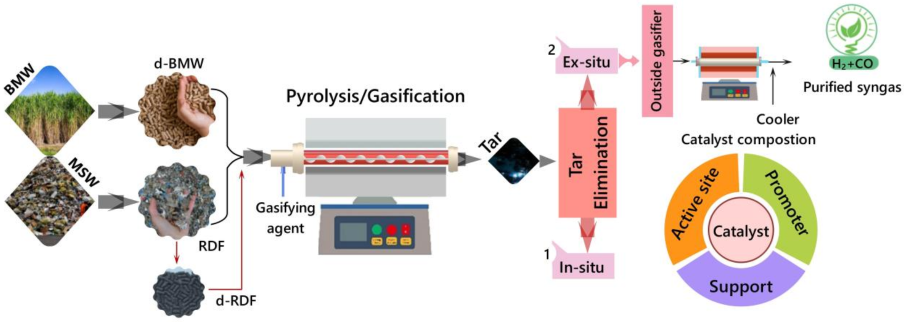
Graphical abstract



Abstract

The formation of tar presents a major obstacle to the advancement of densified refuse-derived fuel (d-RDF) pyrolysis/gasification technologies, highlighting the efficient tar conversion strategies critically important. Catalytic tar reforming has emerged as a prominent technique for improving the efficiency of d-RDF gasification. Using activated carbon (AC), with abundant pore structure, high surface area, and unique chemical properties demonstrated an efficient potential as a support in tar conversion, enhancing resource application and system efficiency. However, catalyst deactivation is a widespread issue that remains a key challenge in catalytic tar conversion, significantly limiting its industrial application. This paper investigates AC modification, activation, catalytic performance in tar reforming, deactivation mechanisms, and regeneration strategies. The ex-situ catalytic performance of the catalysts was evaluated at various reaction temperatures using a two-stage fixed-bed reactor. The Ni/AC catalyst, with a specific surface area of 925.06 m^2/g, demonstrated promising performance. As the catalyst loading increased from 0 to 18 g, the tar content was significantly reduced from 15 g/Nm^3 to 2.1 g/Nm^3, achieving a high tar conversion efficiency of 85 % at a catalytic reaction temperature of 800 °C. H_2 was the dominant gas in the product gas, likely due to the enhanced cracking and reforming reactions of tar facilitated by the catalysts. The total gas yield reached 53.5 %, with a lower heating value (LHV) of 12 MJ/Nm^3, H_2 yield of 13 mol/kg d-RDF, and a CO yield of 2.9 mol/kg d-RDF. In comparison to previous studies, the Ni/AC catalyst demonstrated competitive performance in terms of tar conversion efficiency. However, despite these advancements, sintering and coke deposition remain significant challenges in catalytic conversion of tar, necessitating improved modification strategies to enhance catalyst stability and activity.

Keywords: gasification, tar formation, catalyst, ex-situ tar conversion.

Magnesium Recovery from Brine via Reactive Membrane Crystallization Using Hollow-Fiber Modules

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Key words: magnesium recovery, ion-exchange, membrane crystallization

Drinking water supplies are decreasing in some coastal areas, making it necessary to seek alternative solutions for potable water production. One approach to alternative solutions is the concept of circular economy, which aims at the recycling and regeneration of water resources. One such alternative is seawater desalination using reverse osmosis. However, desalination generates vast amounts of highly concentrated waste streams, known as brine, which are currently discharged back into the ocean. This waste stream contains almost twice the salt concentration of seawater, making it an untapped source of critical raw materials for the European Union. By processing this brine, it would be possible to produce valuable materials while also obtaining clean water. One of these valuable materials is magnesium, which can be separated by reactive crystallization through the addition of a precipitating agent.

Our goal is to separate magnesium from brine using membrane technologies. Membrane crystallization enables the controlled introduction of the precipitating agent without direct contact between the two solutions, resulting in a more easily controllable process. This process employs ion-exchange membranes in the form of hollow fibers. The membrane crystallization was conducted using a membrane module composed of a fiber wounded around a 3D-printed body, which was immersed in a model $MgCl_2$ solution. The experiments were carried out with NaOH as the precipitating agent. The possibilities of increasing the yield after crystallization were investigated through the addition of HCl, osmotic water permeation, and aeration. Subsequently, pilot membrane crystallization experiments were performed using a multi-fiber membrane module, whose construction resembles a shell-and-tube heat exchanger.

Acknowledgments

This work was supported by the Slovak Scientific Agency, Grant No. VEGA 1/0658/24, and the Slovak Research and Development Agency under the contract No. APVV-22-0038 and VV-MVP-24-0365.

Optimization of Thermochemical Conversion Feedstock Parameters for an Integrated Waste (Bio)refinery

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Waste generation is a growing environmental problem that requires ideas and new research for its solution. Energy and material recovery are suitable for mixed waste, which cannot be recycled easily. To increase the total conversion and efficiency of mixed waste processing, it is necessary to integrate several waste treatment methods, creating an integrated waste (bio)refinery. Thermochemical conversion unit, i.e. gasification process, is an integral part of such (bio)refinery. Gasification unit is suitable mainly for processing of residual waste streams with low moisture content and high calorific value, such as refuse-derived fuel (RDF) or lignocellulosic biomass. Feedstock for the gasification in an integrated waste (bio)refinery contains a mixture of waste types combined with the waste streams from different processing units in the (bio)refinery. The main challenge in processing such feedstock is its always changing composition, which implies the changing properties of products and operating conditions. Therefore, this work investigates optimization methods to achieve constant parameters for the mixed gasification feedstock. This is done by changing the ratios of different components in the feedstock. Feedstock for gasification in an integrated waste (bio)refinery typically consists of RDFs from municipal solid waste and mixed plastic waste, lignocellulosic biomass, solid residue from biological waste treatment in the (bio)refinery (e.g. digestate from anaerobic digestion) and various waste streams generated in the (bio)refinery. The most important parameters of the mixed feedstock for thermochemical conversion, which have to be fixed, are heating value, moisture and ash content, concentrations of S, N and Cl contaminants and ratios between oxygen, hydrogen and carbon. Mathematical model was developed in MATLAB environment, which optimizes the amounts of lignocellulosic biomass and RDF from plastic waste in the mixed feedstock. It was confirmed that using this method it is possible to fix the parameters of the feedstock to desired values. This is very important to ensure the smooth operation of the gasification unit and production of the desired products.

Keywords: waste biorefinery; gasification; feedstock optimization

Acknowledgement:
This work was supported by the Slovak Research and Development Agency under the contract No. APVV-19-0170 and by the program for supporting young researchers funded by the Slovak University of Technology.

Reuse of quaternary treated wastewater for agricultural irrigation, reality or fantasy?

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Key words: crops, irrigation, quaternary water treatment, wastewater reuse

Abstract

Human activities significantly impact environmental conditions, leading to challenges such as biodiversity loss and water scarcity, particularly manifested through increased water stress. One promising solution to mitigate these challenges is the reuse of treated wastewater (TWW) for agricultural irrigation. However, using TWW for this purpose raises concerns regarding soil quality, crop health, and consumer safety. This study explored a quaternary wastewater treatment process employed at a wastewater treatment plant (WWTP) in Trnava at Zeleneč, Slovakia, with purpose of making the TWW safe for irrigation, while monitoring the water, soil and crop quality. For the purpose of the study, various agricultural crops, including onions, potatoes, carrots, and parsley were grown by using quaternary treated wastewater. The study implemented advanced water treatment methods such as coagulation, ultrafiltration, adsorption, and disinfection to elevate the quality of treated wastewater. The results demonstrated a significant improvement in the quality of the treated wastewater, indicating its suitability for agricultural use. Specifically, there was a reduction in chemical oxygen demand (COD) from 34.5 mg/L in the raw effluent to 24.5 mg/L post–treatment, representing a removal efficiency of 63%. Regarding nitrogen, TN and it's the effect of quaternary wastewater treatment was also assessed for pharmaceuticals and drugs, which showed remarkable reduction of 99.2% for methamphetamine and over 50% removal efficiency for additional pharmaceuticals detected in the raw WWTP effluent. Importantly, no harmful antibiotic residues were found in the quaternary treated wastewater, confirming that the treatment process effectively mitigated potential health risks associated with the use of wastewater in agriculture. These findings suggest that treated wastewater is a viable option for sustainable agricultural practices, enhancing food safety and addressing water scarcity issues.

Start your research with LRI ENREGAT!

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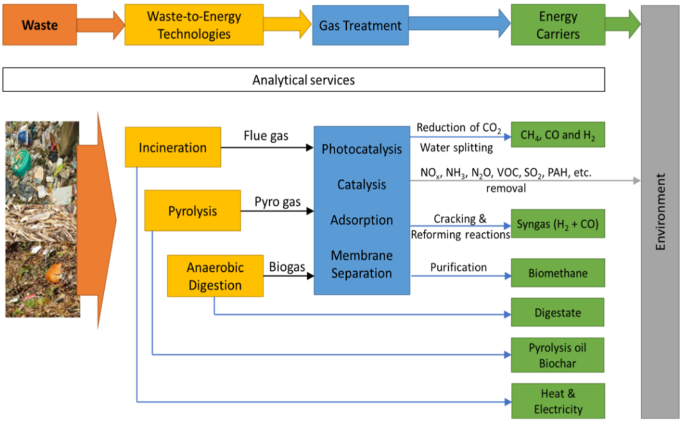
Keywords: large research infrastructure, open access

The ENREGAT large research infrastructure, a unique platform for comprehensive research on material and energy waste recovery through combustion, pyrolysis, anaerobic processes, and gas treatment using (photo)catalytic and other advanced methods, has been providing free open access to the global scientific community for the seventh year, thanks to funding from the Ministry of Education, Youth, and Sports (Project No. LM2023056).
What sets ENREGAT apart is its ability to conduct both fundamental and applied research, from lab-scale to pilot-scale, enabling efficient evaluation of the best technologies for specific waste types.
To date, over 500 open-access applications have been approved from universities worldwide. ENREGAT is also a key partner for researchers from the Czech and Slovak Academies of Sciences. Through collaborative and contractual research, ENREGAT bridges science and industry, turning research into sustainable solutions with economic and societal impact. Its contributions include 120+ high-impact journal publications, 20+ applied research breakthroughs and 70+ successfully defended student final theses.



Acknowledgments. Financial support from MEYS, project No. LM2023056 is acknowledged.

Lectures: Energy transition and circular economy

Comparison between Ni/ZSM-5 and NiMo/Al_2O_3 Catalysts in the Hydrocracking of Fischer–Tropsch Wax – Reflected in the Properties of Middle Distillates

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Key words: hydrocracking, Ni/ZSM-5, NiMo/Al_2O_3, Fischer-Tropsch wax, middle distillates

The harmful emissions caused by fossil fuels have long been recognized as a major issue. Various actions have been implemented worldwide to mitigate these negative effects. In the European Union, the ReFuel EU regulation and the RED III directive have been introduced. Both regulations promote the use of so-called e-fuels. This fuel category includes gasoline and middle distillates produced by Fischer-Tropsch synthesis from hydrogen generated using renewable electricity and carbon monoxide derived from renewable sources. In the low-temperature variant of the synthesis, which is more favorable from the perspective of middle distillate production, a large quantity of a low-value, high molecular weight paraffin fraction—known as Fischer-Tropsch wax—is formed. The conversion of this fraction has been considered crucial for the yield of hydrocarbons within the fuel boiling range and thus for the overall economic viability of the process. Fischer-Tropsch waxes have most commonly been subjected to some form of cracking. In terms of middle distillate quality, it has been found advantageous to perform hydrocracking, as the resulting fractions mainly consist of saturated hydrocarbons. In contrast, when thermo-catalytic cracking is carried out without a hydrogen atmosphere, the products have been found to contain a high proportion of olefins and aromatics. A high content of saturated hydrocarbons has been associated with improved stability, an increase in the smoke point for JET fuels, and an improvement in the cetane number for diesel gas oils. During our experiments, the hydrocracking of Fischer-Tropsch wax was carried out using two different commercially available nickel-containing catalysts in a continuous, single-pass, back-mixing-free microreactor system. The influence of the catalysts and changes in operating parameters on the yield and composition of the products was investigated. In addition, several key properties of the middle distillates were determined, including density, cold flow properties, and distillation characteristics. It was found that increasing the temperature and residence time improved the cold flow properties of the obtained middle distillates.

This work has been implemented by the TKP2021-NKTA-21 project with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the 2021 Thematic Excellence Programme funding scheme.

Hydrogen Position in the Energy Transition: Analysing the Competitiveness of Low-Emission Technologies

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Key words: hydrogen energy, transportation, multi-criteria evaluation.

The role of hydrogen as a clean energy carrier is gaining growing attention in the context of achieving climate neutrality and decarbonizing key sectors of the economy. While hydrogen has already found its place in various industrial processes, its potential extends far beyond traditional applications. Viability of low-emission hydrogen technologies within the broader energy transition is provide by this study, focusing not only on production, but also on other parts of hydrogen supply chain such as transportation and end-use. A comparative analysis is conducted based on several criteria: economic feasibility, environmental performance, technical parameters and technological maturity.

The study also accounts for dynamic variables such as projected energy prices, carbon costs, and efficiency improvements, which can significantly influence the future competitiveness of hydrogen application pathways. The results provide a data-driven evaluation of low-emission hydrogen options and identify the most promising applications in both the energy and industrial sectors. The results highlight its prospects compared to conventional technologies. The role of hydrogen transport is also applied in this study as part of the comparison of the offered options. This contribution aims to provide relevant insights into the role of hydrogen in the energy transition and inform strategic decisions regarding future investments.

Acknowledgement

This work was supported by the call for doctoral students and young researchers of Slovak University of Technology in Bratislava to start a research career (Grant 23-04-11-A) and by the Slovak Scientific Agency, grant no. VEGA 1/0151/24.

IMPLEMENTATION OF DESALINATION TECHNOLOGY IN AMMONIUM THIOSULFATE MANUFACTURING

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Ammonium thiosulfate (ATS) is an inorganic compound with applications in agriculture, particularly as a fertilizer. Its production process generates substantial waste heat, which can be used for seawater desalination, an especially valuable resource in regions dependent on desalinated drinking water.

This study explores two methods for utilizing ATS-derived heat in desalination:

Direct thermal desalination, where steam from ATS production drives evaporation in a brine evaporator and indirect power generation, where steam turbines convert waste heat into electricity to operate reverse osmosis (RO) systems.

The analysis evaluates thermal efficiency, energy consumption, and water recovery rates for both approaches, comparing their advantages and limitations. While evaporative desalination leverages steam for boiling seawater, the RO method relies on turbine-generated electricity to power high-pressure pumps. The objective is to determine the most energy-efficient integration, minimizing waste while enhancing desalination output. Findings provide a technical and environmental assessment of coupling ATS production with desalination, exploring options to improve sustainability in water-scarce regions.

The authors acknowledge the financial support from the Slovak Society of Chemical Engineering. This study was supported by the Slovak Research and Development Agency under contract no. VV-MVP-24-0365.

Modelling metal deposition on a 3D electrode in a hybrid flow battery: Validation by microcomputed tomography imaging

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Key words: Hybrid redox flow batteries, modelling, micro-computed tomography

While a number of subtypes of redox flow batteries (RFBs) have already been successfully commercialized, hybrid flow batteries (HFBs) still have unresolved challenges. The main difference, setting this subtype apart from most RFBs, is that deposition of metal is required at one of the electrodes. The common issue is, that the metal deposition is uneven across the electrode. This can lead to a host of performance issues, lesser areal capacity during cycling and in some cases even mechanical damage to the cell, shortening its lifespan. To address these issues, mathematical modelling can be employed. It can be powerful tool for understanding the complex process of metal deposition and optimization of the operating parameters of HFBs, which could lead to more uniform deposited metal distribution. However, validation of such model is challenging.

To address this issue, we have developed a macro-homogenous model, which is able to predict the dynamic evolution of the deposited metal distribution. We subsequently validated the model predictions using online pressure drop and conductivity measurements as well as spatial metal distribution obtained from imaging techniques, including 3D micro-computed tomography. The model is based on a zinc-iodine hybrid flow battery with a 3D porous negative electrode. In the proposed model, the 3D electrode is characterized by locally distributed porosity and conductivity which evolve in time along with the amount of deposited metal. Experimental data (felt electrode compression rate, current flow, pressure drop) and 3D micro-computed tomography porosity estimates, all sourced from our previous papers [1, 2], were used as input parameters to the model.

So far, the model results agree with general trends of the metal deposition data, but further optimization of the model will be needed for better results. In the future, the developed model will be suitable for simulation of a wide range of HFB chemistries based on electrodeposition, further advancing the ability of energy storage producers to optimize flow battery (FB) systems.

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Lectures: Process design and process intensification

Production of carboxylic acids from organic waste via electro-fermentation: selectivity, recovery and electrochemical upgrading opportunities

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Key words: carboxylic acid, dark fermentation, electro-fermentation, oxidative decarboxylation

Transforming organic waste into useful recoverable products is a challenging issue, which requires highly efficient and integrated technological solutions to obtain value-added resources. In this work, the organic waste-based production of carboxylic acids (CAs) via electrochemically assisted dark fermentation was studied. Compared to conventional dark fermentation, electro-fermentation applies an external reducing power to achieve ‘unbalanced fermentation’, resulting mainly in shifts in product selectivity, yields and kinetics. During the treatment of kitchen waste, electro-fermentation proved to be advantageous in terms of improving chain elongation to caproic acid (C6) at higher organic loads. In addition, the lag-phase during electro-fermentation was significantly reduced compared to the conventional dark fermentation. Microbial consortia analysis of the bulk revealed that although higher caproic acid production occurred during electro-fermentation, C6-related bacteria were present with lower relative abundance, indicating remarkable fermentation efficiency improvement, assumably together with lower biomass yield.

The produced CAs – after separation and concentration by e.g. (bipolar) electrodialysis – can be directly used, or further upgraded to higher-value components. Recently, electrochemical methods gained attention, since those fit well to the trends of electrifying biotechnology. This study assessed the potential of electrochemical upgrading via anodic decarboxylation and dimerization. In this process, the decarboxylated CA radicals can form dimers, resulting in alkanes – e.g. decane from caproic acid (C6) -, or could undergo other pathways, forming esters, alcohols, short alkenes, etc. Using model solutions of pure CAs and mixtures, mainly alkanes and esters were obtained, with increased selectivity to alkanes with longer chain CAs.

In summary, it was shown that both the fermentation, separation and upgrading of the CAs can be improved by using electrochemical approaches, thus allowing efficient waste-to-product processes.

This work was supported by the 2024-2.1.1-EKÖP University Research Fellowship Program of the Ministry of Culture and Innovation from the source of the National Research Development and Innovation Fund.

Lectures: Digitalization and process control

Chemical process response analysis to single and multiple input parameter deviations.

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Key words: nonlinear system; hazard identification

Nowadays the chemical industry uses more complex processes. These processes produce complex products and need to decrease emissions emitting and energy consumption. These processes require more sophisticated equipment and interconnected units. Meeting these demands presents challenges in design, control, analysis, process safety, and economics. Chemical process behavior is basically nonlinear, as demonstrated during malfunctions, which lead to changes in operating parameters. Nonlinear behavior can occur in whole working range of input parameters, it can occur in specific range of parameters or under specific conditions or combination of input parameters. In some cases, nonlinear response is observed in other pieces of equipment of unit or other plant connected to plant with change in input parameters. Nonlinear behavior caused by interactions between independent parameters is hardly predictable and can be overlooked during hazard analysis, e.g. HAZOP. Response of nonlinear system can by manifested by oscillatory behavior, domino effects or high sensitivity to change in input parameters (fast change in temperature, pressure or runaway effect). Identification of nonlinear behavior to deviation of design input parameters can be done at equipment, where deviation appears but also at connected equipment and units. Including connected units to analysis has additional value in identifying domino effects or consequence effects, which can occur only on other units than the original unit of deviation. Including mathematical modeling to hazard analysis like HAZOP can increase the number of identified potentially dangerous scenarios, which are manifestations of nonlinear system behavior.

Process response to single input parameter deviations is analyzed by nonlinearity measures (NLM) (Helbig et al., 2000). NLM is suitable to analyze nonlinear response of system in chosen range of deviation values, all possible values of deviated parameter or to identify ranges, where is nonlinear behavior strongest. Morris (1991) sensitivity analysis is used to evaluate system response to multi-input parameter deviations. This method provides two information about each analyzed input. The first information is influence at system response and the second information is nonlinear effect and/or interaction with other analyzed inputs. Propylene glycol production is chosen as case study for single and multiple input parameter deviations. The chemical plant consists of a continue stirred tank reactor and two distillation columns. It was modelled with Aspen Plus Dynamics® and Matlab®. Parameters used for analysis were propylene oxide flow, water flow, cooling water temperature and cooling water flow. The analyzed process response was temperature of reactor and temperature of condenser and reboiler of both columns. The strongest nonlinearity was observed due to water flow deviation, which showed the highest NLM values. These results are compatible with Morris analysis results, which identify water flow deviations as deviations with strong nonlinear behavior and/or interactions and also they have significant influence on temperature.

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Reinforcement learning for chemical process control

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Key words: reinforcement learning, chemical process control, multi-agent reinforcement learning, resilience engineering, explainable reinforcement learning

Reinforcement learning (RL) algorithms are well-suited for sequential decision-making tasks, making them an excellent choice for chemical process control, where making decisions is required continuously. In this paper, we explore the application of RL at different levels of hierarchical process control to assess its potential to improve efficiency and robustness. We present two case studies of chemical process control applications, one with resilience engineering and explainable reinforcement learning, and one with multi-agent reinforcement learning. In the first case study, an intervention action is designed with RL to prevent reactor runaway in a batch reactor, and resilience is applied as a reward function. Two explainable reinforcement learning methods are investigated, a decision tree, as a policy-explainer, and the Shapley value as a state-explainer. The decision boundary of the decision tree is compared with the runaway boundaries defined by runaway criteria, and the Shapley value explains how different state variables influence the agent's decisions over time. The results show that this method is applicable to the developement of a resilience-based mitigation system, and can be explained and presented transparently. In the second case study, two RL controllers are applied, one RL controller varies the feed rate in the feed phase of a semi-batch reactor, while the other RL controller in the mixing phase works as a master controller in a cascade control structure. The multi-agent structure enables the handling of more complex chemical processes beyond the capabilities of a single agent. The developed RL controllers perform effectively and can keep the temperature at the desired setpoint.

Acknowledgement
This work has been prepared with the professional support of the Co-operative Doctoral Program of the University Research Scholarship Program of the Ministry of Culture and Innovation financed from the National Research, Development and Innovation Fund. The work was supported by the 2024-2.1.1-EKÖP University Research Scholarship Programme of the Ministry for Culture and Innovation from the Source of the National Research, Development and Innovation Fund.

Why we waste the time of educated people on trivial activities - how to know more by doing less

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The aim of the presentation is to present the limitations in the work of scientists resulting from the traditional organization of the synthesis laboratory and the lack of continuous monitoring of reactions and conducted processes. Most of the work requires many manual activities without providing answers - data for scientific considerations. At the same time will be presented the possibilities of increasing the efficiency and effectiveness of conducted research and effective use of the most important attribute of a scientist - his mind.

The main limitations of scientists when conducting reactions are:

- incomplete possibility of reaction control and uncertainty as to the actual impact of individual process parameters,
- necessary presence of staff to change parameters and register events, which may pose a health risk, and at the same time limits the number of experiments performed
- the need to wait for the results of off-line analyses to learn the results of the experiment

In a modern laboratory, the researcher can conduct much more successful synthesis, reducing the time (and number of experiments) needed to complete the research. And the time and data obtained can be used to ask the right questions:

- what happened?
- what did not happen?
- why?
- what to change to make it happen?

Lectures: Separation processes and transport phenomena

Enzyme synthesis and continuous flow separation of (R)-1-phenylethanol in a modular microfluidic system

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Key words: (R)-1-phenylethanol, Continuous flow production, Microfluidics, Enantiomer

The synthesis of enantiomerically pure compounds remains a key challenge in chemical engineering, particularly for industrial applications. Microfluidic systems, which significantly enhance reaction and transport processes, offer a promising approach to overcoming this challenge. In this study, we present a modular microfluidic platform designed for the continuous production of (R)-(+)-1-phenylethanol (R-PE) from racemic 1-phenylethyl acetate (PEAc). The system integrates a packed-bed reactor (PBR) with immobilized lipase for enantioselective hydrolysis and a slug flow extractor (SFE) for efficient removal of unreacted substrate using hexane. Kinetic analysis of the enzymatic process revealed competitive inhibition by R-PE, while extraction studies provided insights into separation efficiency and mass transfer characteristics. By optimizing residence times in both modules, we achieved nearly 90% yield of R-PE within a total reaction time of 260 s - up to 100 times faster than conventional batch reactors. Our results demonstrate how precise kinetic and transport data can be leveraged to design efficient continuous-flow processes for the rapid production of optically active compounds.

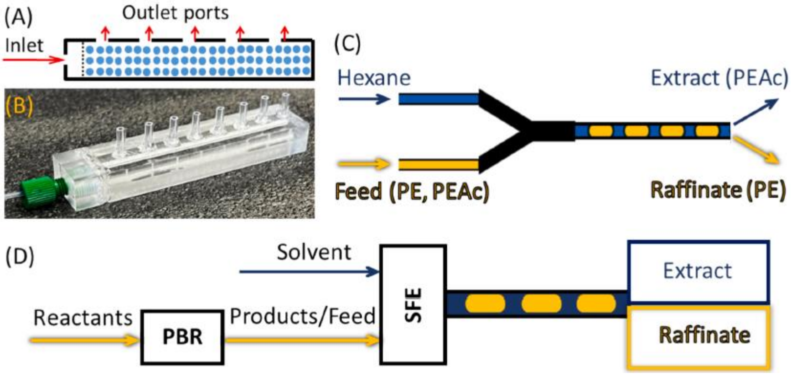

Fig. 1: A scheme (A) and photo (B) of PBR, a scheme of SFE (C), a scheme of the modular microfluidic system (D).

Green analytical strategies for selenium determination using both chromatographic and spectrometric methods

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Key words: green analytical chemistry, selenium determination, oxygen flask combustion, chromatography, spectrometry, piazselenol, fluorescence

Selenium is an essential trace element in animals and humans. Compared to other micronutrients, there is a much narrower range between the normal concentration and the toxic amount of selenium in living organisms. The inorganic forms of selenium (selenate, selenite) present up to 40 times higher toxicity than the organic species (*e.g.* selenocysteine, selenomethionine). Due to these considerations, a sensitive method is required for detection of selenium compounds in biological samples.

Development of greener, more sustainable, and ecofriendly methods for sample decomposition coupled with advanced miniaturised analytical techniques are future promising scientific activities for analytical chemistry. Although less explored recently, methods based on combustion with oxygen are excellent alternatives with potential great superiority over classical strong acids and oxidants-based sample digestion methods due to its high greenness degree, simplicity, speed, sample size and safety. Since the combustion takes place in a completely closed system, no analyte is lost, even the most volatile ones and the interference of organic matter is completely inexistent because the combustion takes place at very high temperatures.

In the present work, a simple and green version for oxygen rich combustion sample dissolution method using an oxygen flask prefilled with oxygen and a platinum-based catalyst is used for the decomposition of food type certified reference samples. Following this step, the samples are analysed using a small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry. For the validation of this method, other previously known methods—fluoresence spectrometry and high performance liquid chromatography—that have been employed as well.

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, contract nr. 15PED/2025, project number PN-IV-P7-7.1-PED-2024-0091, within PNCDI IV

Intensification of Separation Processes in a Model Electrodialysis Unit

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Keywords: electrodialysis, concentration polarization, desalination, electroconvection, gravitational convection, side stream recovery, flow-through cell

Electrodialysis (ED) is a promising electromembrane technique used for selective ion separation, particularly in water desalination and resource recovery. However, its performance is often limited by concentration polarization and the associated electric resistance near ion-exchange membranes. Our recent studies suggest that natural convection, driven by solute-induced density gradients, can effectively mitigate polarization effects even under underlimiting conditions. We confirmed the dominant role of natural convection in model ED channels by measuring concentration profiles in the diluate stream, which showed significant vertical variations: desalted and highly concentrated solutions were withdrawn from the top of the diluate and the bottom of the concentrate channels, respectively.

This accumulation of desalted solution at the top naturally suggests implementing side withdrawal streams for its recovery, whereas similar bottom-side streams can recover highly concentrated solution. Our research therefore focusses on the development and experimental evaluation of a model electrodialysis unit designed to promote natural convection and enable the recovery of additional streams through side ports. We constructed a novel flow-through ED cell that comprises a central diluate channel and two concentrate channels, each equipped with additional strategically positioned side outlets. Cell geometry was optimised through preliminary 2D numerical simulations and practical experiments to promote natural convection.

Experimental characterisation was performed using NaCl solutions at various flow rates through the additional side ports and at various applied currents. The system was evaluated by measuring the concentration and voltage with continuous sampling of diluate or concentrate through the side ports. The results confirmed the possibility of the withdrawal of the desalted and concentrated solutions accumulated at the top and bottom of the flow-through channels. These side streams exhibited enhanced separation efficiency without the need for overlimiting voltages or turbulizing spacers.

Ion concentration polarization for separation of charged species

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Key words: ion-exchange membranes, concentration polarization, overlimiting current, ion separation, Poisson-Nernst-Planck-Navier-Stokes model

Polarization of ion-exchange membranes in a DC electric field leads to the formation of ion-depleted and ion-concentrated zones in the solution layers adjacent to the membranes. The ion-depleted zone is especially interesting owing to a multitude of reaction-transport phenomena associated with its occurrence. Although not apparent immediately, such a zone offers auspicious conditions for controlling the transport of ionic species present in the surrounding solution. To shed light on the working principle of such systems, we analyze the system behavior theoretically with a 2D model based on the Poisson-Nernst-Planck-Navier-Stokes set of equations and confirm its prediction experimentally by conducting a study looking into the behavior of charged chemical species differing primarily in their charge number. Specifically, we show that the ion-depleted zone works as a nonmechanical filter that displays ion selectivity if the separated ions differ in their electrophoretic mobility, affected mainly by the charge number and diffusion coefficient. This selectivity is given by differing electrophoretic forces acting on individual ionic species. The talk will focus on elucidating the fundamental principles governing the studied system and show its use for pseudo-continuous separation of charged dyes as a proof-of-principle application.

MATHEMATICAL MODELING OF AN ION TRANSFER IN A DONNAN DIALYSIS PROCESS VIA NERNST-PLANCK EQUATION

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Key words: Donnan dialysis, mathematical modelling, mass transfer

The rising demand, combined with depleting sources of raw materials is forcing the industries to look for an alternative sources of these critical raw materials. One of these alternative sources are concentrated brines, produced in a seawater desalination process, as well as industrial wastewaters containing metal ions. These brines contain substantial amounts of minerals such as lithium and magnesium, which are considered a critical raw resource by the EU. The major problem with this source is the complexity of this mixture, containing a wide variety of ions, and requiring a specialized approach for recovery of the compounds of interest. One of relatively new approaches capable of achieving this is a membrane crystallization utilizing ion exchange membranes. In this process an ion of interest is transported across the ion exchange membrane via a Donnan dialysis process after which it is reacted with a suitable precipitant resulting in the formation of crystalline phase. In this process the mass transfer across the membrane via a Donnan dialysis is a key step determining the rate of the process.

One of the key tools required for an effective development of a new process is a suitable mathematical model capable of describing the systems and phenomena taking place in these systems. The objective of this study is to compare and verify some of the approaches for description of the Donnan dialysis process found in literature. These tested approaches are based on various simplifications of a Nernst-Planck equation. After determining of the required parameters, the four different models were verified against an experimental data of ion transport across an anion exchange membrane under different conditions. The results highlight the importance of selection of a suitable model for description of these systems.

Acknowledgement*:*
This work was supported by the Slovak Scientific Agency, Grant No. VEGA 1/0658/24, and the Slovak Research and Development Agency under the contract No. APVV-22-0038 and VV-MVP-24-0365.

Reaction transport phenomena at ion-exchange membranes in DC electric field

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Keywords: electrodialysis, concentration polarization, desalination, electroconvection, gravitational convection

The global challenge of ensuring safe drinking water spans from desalinating seawater and brackish water in coastal regions to treating polluted freshwater sources. Membrane processes are crucial in tackling these issues, with reverse osmosis being the primary method for conventional water desalination. However, electromembrane technologies, particularly electrodialysis, are emerging as viable alternatives, especially for smaller desalination plants and industrial applications focusing on producing ultrapure water rather than potable water.

Despite its promise, electrodialysis is limited by concentration polarization, an intrinsic phenomenon that occurs on membranes under DC bias. Gaining deeper insight into the reaction-transport phenomena behind this effect is necessary for designing and optimizing more efficient electrodialysis systems. Interestingly, solute-induced gravitational convention has emerged as a potential solution to at least partially mitigate the challenges posed by concentration polarization.

Our research aims to enhance the understanding of phenomena occurring on ion-exchange membranes through both experimental and theoretical approaches. To investigate the mechanisms at play, we designed, constructed, and utilized an electrochemical cell for microscopic analysis. Experimental results revealed that gravitational convection initiates immediately in the underlimiting region, significantly influencing mass transfer along the ion-exchange membrane. To support these findings, the second phase of our research involved developing a computational model using COMSOL Multiphysics. We developed a model based on solving the Navier-Stokes, Poisson, and molar balance equations, enabling the prediction of both natural convection and electroconvective vortices. The model demonstrated that natural convection can significantly impact mass transport along the ion-exchange membrane.

Application of genetic algorithm for multiparametric optimization of double reactor membrane hybrid systems

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Key words: biotransformation, phenylacetaldehyde, hybrid system, membrane separation, genetic algorithm, optimization

In many biotransformation productions product inhibition of a production strain strongly decreases the yield and the effectivity of the process. To overcome this an in-situ removal of the product from the fermentation medium is necessary to apply. Application of membrane bioreactors with immersed or external capillary membrane module are the promising solution for this case used in many applications in recent years. Membrane bioreactors combine production and separation processes to one production system, hybrid system, to increase thus the bioreactor productivity or productivity of the whole production line. Good example is the bioproduction of natural aromas in hybrid system such as 2-phenylethanol produced from amino acid L-phenylalanine catalysed by yeasts *Saccharomyces cerevisiae*. 2-Phenylethanol is well known rose aroma and can be further utilized as a substrate by oxidative bacteria such as *Gluconobacter oxydans* to phenylacetaldehyde. 2-Penylethanol and phenylacetaldehyde are valuable components of flavours and its natural production is of interest in the flavour, pharmaceutical and food industry nowadays.

In this work the multiparametric optimization of bioproduction of phenylacetaldehyde directly from the substrate L-phenylalanine through the intermediate 2-phenylethanol is presented. Optimization was performed for four types of double reactor membrane hybrid systems incorporating membrane separation based on pertraction and membrane extraction using immersed or external membrane module. Based on the genetic algorithms and the economy of the process the setting of nine operative parameters of hybrid system (such as membrane area and medium flow rates of the membrane modules, glucose feeding rate, biomass concentration or volume of fermentation medium in second bioreactor) was optimised and compared to reach the highest operational profit. To reach the best results for optimalization due to the limitations of the computing technique the optimization of the genetic algorithm parameters was also carried out.

Acknowledgement: This work was supported by the Slovak Grant Agency, grant VEGA 1/0548/21.

Use of multifiber membrane module for lithium recovery

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Key words: multifiber module, Donnan dialysis, lithium

Lithium is considered a highly valuable substance not only because its extraction is challenging but also due to its limited availability on land. According to lithium consumption forecasts, by 2050, up to one-third of the lithium reserves that can be extracted from terrestrial sources are expected to be depleted. Up to 65% of the produced lithium is used in batteries, and this percentage is expected to increase in the coming years due to electrification. It will be necessary to expand recycling capacity of Li-ion batteries due to increasing electrification, considering only 5% of used batteries were recycled in 2022. This process generates several waste streams, which still contain enough lithium that can be separated. The experiments were carried out using a model solution composition that corresponds to the brine produced during battery recycling. This solution mainly contains lithium cations and chloride anions, which together form a highly soluble mixture. To reduce the solubility of lithium, the solution was converted into lithium bicarbonate using anion-exchange hollow fibers. Lithium bicarbonate is still well soluble, but by heating to temperatures up to 80°C, it transforms into poorly soluble and commercially most valued lithium carbonate. The resulting crystals were analyzed for crystal size distribution. The conversion of lithium chloride solution into lithium bicarbonate was performed in a multi-fiber module packed with anion-exchange fibers manufactured by MemBrain s.r.o. The experimental investigation was focused on the influence of different packing densities on Donnan dialysis, as well as on effect of hydrodynamic conditions on the rate of mass transfer. Since Donnan dialysis is a time-consuming process, it was necessary to examine lithium losses during the experiments. The results showed that lithium losses through the membrane cannot be significantly influenced by changes in operating parameters, as they primarily depend on the concentration of functional groups in the membrane. However, what could be influenced by changing the process conditions was the rate of anion exchange, which was strongly affected by temperature. Flow rates inside the fibers and in the shell of the module influenced the transmembrane pressure, which during longer experiments led to a significant amount of water passing through the membrane, which was an undesirable effect in our case.

Acknowledgments

This work was supported by the Slovak Scientific Agency, Grant No. VEGA 1/0658/24, and the Slovak Research and Development Agency under the contract No. APVV-22-0038 and VV-MVP-24-0365.

Lectures: Pharmaceutical engineering and processes

An Introduction to the Stochastic Nature of Nucleation in Freeze-Drying

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Keywords: freeze-drying, freezing step, nucleation temperature, stochastic nucleation

The stochastic nature of nucleation is often considered a limitation in the freeze-drying process, as it introduces variability that can affect both product quality and process efficiency. Since nucleation occurs at different temperatures and times, it influences the size of ice crystals, which in turn affects the sublimation rate and the porous structure of the final product. Non-uniform nucleation can prolong drying time, increase energy costs, and impair product rehydration. Additionally, products with varying structures may exhibit different physicochemical properties, which is particularly critical in the pharmaceutical and food industries. Various methods have been developed to mitigate this issue; however, the underlying mechanisms of nucleation stochasticity remain poorly understood. This study aims to introduce the problem of stochasticity and identify the key factors contributing to heterogeneity. The tested factors include sample volume, solution composition, and vial positioning. All of these factors were found to influence nucleation stochasticity.

Computational insight to observed collective phenomena of lipid membrane permeation

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Keywords: phospholipid bilayer, molecular dynamics, permeation, 5(6)-carboxyfluorescein

The permeation of a substance through the phospholipid bilayer is a key factor in drug transport to its site of action. This ability is quantitatively expressed as a permeability coefficient and can be experimentally determined using various methods. One such is a liposomal leakage assay.

In previous experiments[1], this assay was used to measure the permeability of 5(6)-carboxyfluorescein (CF), taking advantage of its self-quenching properties at high concentrations. However, when another drug molecule was encapsulated in liposomes alongside the CF, its permeation profile changed. This was unexpected, as permeability of a molecule was so far determined solely by the phospholipid bilayer and the molecule itself.

These results indicate that the presence of an additional molecule type alters the permeability of CF, potentially due to interactions between the drug and CF or between the drug and the phospholipid membrane. Such interactions may either facilitate or hinder the passive transport of CF, thereby influencing the overall permeability profile. To gain deeper insight into the molecular mechanisms underlying these observations, we employed molecular dynamics (MD) simulations, which are widely used in contexts where understanding atomic-level interactions is crucial, such as in molecular docking.

Our MD simulations have so far explored interactions between the drug and the lipid membrane or CF and the lipid membrane. These simulations were conducted under a heating and cooling protocol designed to mimic conditions during molecular loading. The results have provided insights into the tendency of the drug molecule to incorporate into the lipid bilayer and its propensity for molecular clustering—both of which will help explain experimentally observed phenomena.

[1] Odehnalová, K.; Balouch, M.; et al. Liposomal Copermeation Assay Reveals Unexpected Membrane Interactions of Commonly Prescribed Drugs. *Molecular Pharmaceutics* **2024**, *21/6*, 2673–2683. DOI: 10.1021/acs.molpharmaceut.3c00766.

Development and Optimization of a Continuous Liquid Antisolvent Precipitation Device for Nanocrystalline Formulations

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Key words: Antisolvent precipitation, Nanocrystals, Continuous processing, High-throughput screening, Optimization, API solubility

The increasing number of poorly water-soluble active pharmaceutical ingredients (APIs) presents significant formulation challenges in early-stage drug development, particularly regarding dissolution rates and bioavailability. Conventional practices that utilise dimethylsulfoxide (DMSO) for preclinical studies often lead to formulation problems during the clinical phases, highlighting the need for robust, scalable, and direct formulation methods.

This study presents a continuous liquid antisolvent precipitation device (CLAP) designed and optimized for high-throughput production of nanocrystalline API formulations. The CLAP device utilises precise control of solvent and antisolvent streams to produce stable nanocrystals with enhanced solubility and bioavailability. A modular design that incorporates interchangeable mixing chambers, HPLC grade pumps, and automated parameter control was implemented to facilitate rapid experimentation and scalability.

Extensive parametric studies investigated the influence of critical factors such as solvent-to-antisolvent flow ratios, API concentrations, stabiliser types, and mixer geometries on particle size distribution (PSD). Optimal configurations demonstrated the capability to consistently yield nanoparticles below 200 nm with narrow PSDs. Computational fluid dynamics (CFD) modelling and nucleation studies further enhanced understanding of the mixing and nucleation dynamics, guiding mixer design improvements toward achieving minimal particle growth after nucleation.

The developed system provides a platform for early-stage drug screening, reducing the risk of formulation-related development hurdles and accelerating translation from laboratory to clinical application.

Development of advanced methodology for in vitro testing of long-acting injectable depot systems

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Key words: dissolution, methodology, USP-4, injectables, depot, long-acting

Long-acting injectable depot formulations are promising dosage forms capable of controlled drug release over weeks to months, improving patient adherence and stability of therapeutic effect. In clinical practice, the LAIs are injected intramuscularly or subcutaneously and subsequently form a persistent depot, from which active pharmaceutical ingredient (API) slowly releases over a long period of time.

Current dissolution methodologies consist of injecting the formulation into liquid dissolution media and so the depot formation *in vitro* is omitted. Even though these methodologies can provide insight into formulation mechanism of release and pharmacokinetics, *in vitro* introduction of LAI depot formulation and slow absorption into surrounding tissue is critical for better predicting *in vivo* behavior of LAIs based on *in vitro* tests. United States Pharmacopeia apparatus 4 (USP-4) is commonly used for dissolution of long-acting formulations, however it also faces the mentioned shortcomings of the commonly used methods.

The dissolution method currently being developed in this project is based on USP-4 flow-through cell with in-house built adapters. Introduction of hydrogel matrix injected with LAI formulation into the USP-4 cell introduces depot formation and release into surrounding tissue. Hydrogel serves as a mimic of the tissue into which the drug is injected and as a solid but permeable barrier from which the drug gradually diffuses into the surrounding dissolution medium. Of course, hydrogel matrix is only a rough approximation of living tissue, however the results of these modified tests could provide more biorelevant insights than provided by currently used methods.

Drug permeability: commonly misinterpreted bioavailability governing factor

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Key words: permeability, bioavailability, meta-analysis

Permeability is a crucial molecular property in drug discovery that influences pharmacokinetics when drugs cross phospholipid bilayers, such as cell membranes, the gastrointestinal tract, or the blood-brain barrier. Numerous methods exist for determining permeability, including cell line assays (CACO-2, MDCK), cell-free systems like parallel artificial membrane permeability assay (PAMPA), black lipid membrane (BLM), or liposome-based assays. Various *in silico* approaches have also been developed.

We have analyzed already published permeability data (MolMeDB and ChEMBL databases) evaluated four experimental and two computational methods. Results showed poor repeatability even within the same method. For PAMPA, intrinsic and apparent permeabilities can differ by orders of magnitude, suggesting caution when using literature data.

The unstirred water layer permeability (permeability of drug through stationary water layer on the surface of the membrane) causes discrepancies between methods and is often cause of misinterpretation.

Furthermore, we have identified the limitations of studied methods and transferred the hardly imaginable permeability values into real life drug permeation examples which can serve community in order to better interpret both own and literature data. In conclusion, caution is recommended when interpreting or combining permeability data.

Encapsulation in Liposomes and the Critical Role of the Encapsulated Substance

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Key words: drug delivery, liposomes, preparation techniques, encapsulation efficiency

Liposomes are widely used as versatile drug delivery systems, but their preparation methods significantly influence their encapsulation efficiency and physicochemical properties. This study presents a systematic comparison of five conventional liposome preparation techniques: the heating method, the film method with extrusion, the film method with sonication, the freezing-thawing method, and a combination of film method with extrusion and freezing-thawing cycles. Two model substances, 5(6)-carboxyfluorescein (CF) and D-(+)-glucose (GLU), were chosen to examine how different physicochemical properties affect encapsulation efficiency across these methods.

The results demonstrate that the method's effectiveness strongly depends on the physicochemical properties of the encapsulated substance. The film method with extrusion achieved the highest encapsulation for CF, while sonication-based techniques performed better for the more hydrophilic and less permeable GLU. The heating method resulted in highly heterogeneous liposomes with inefficient cholesterol incorporation and the freezing-thawing method showed the lowest encapsulation efficiency in this study.

Furthermore, we observed that encapsulation efficiency in sonication-based methods depends on the concentration of the loading solution, suggesting interactions between the assembling bilayer and the molecules of solute. These findings emphasize that the choice of liposome preparation method should be tailored to the specific physicochemical properties of the encapsulated substance rather than relying on a one-size-fits-all approach.

Experimental and theoretical investigation of spray drying: What can happen in single droplets

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Key words: 3-7 words, spray drying, experimental, theoretical

Spray drying is an important unit operation in pharmaceutical industry to produce solid amorphous dispersions which are frequently used to improve the solubility and thus the bioavailability of poorly soluble active pharmaceutical ingredients. The process can be studied at different levels: droplets, dryers, processes.

Goal of the presentation is to focus on heat and mass transfer phenomena during drying of single droplets. Interesting videos from laboratory ultrasonic levitator showing shrinking, ballooning and exploding of droplets and particles are shown first. Then a detailed distributed parameter model developed for simulation of a single droplet drying is presented. The model describes heat and mass transfer inside the droplet/particle, shrinking of the particle, the skin formation followed by skin thickening, crust formation and the final drying of non-shrinking particle. The model also calculates exchange of heat and mass between the particle and external drying gas and the decreasing particle density. An extension of the model for ballooning and exploding particles is also presented. The models are compared with droplet drying experiments from an ultrasonic levitator.

Multi-physics problems in particulate engineering – 3 case studies

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Industries such as food, pharmaceuticals, chemicals, consumer goods, agriculture, mineral processing as well as advanced materials for healthcare, energy and environment, rely extensively on particle science and engineering. We present 3 case studies that involve coupling the equations of heat transfer, mass transport, chemical reaction, incorporating also the mechanical behaviour in process modelling.

1. Droplet drying is traditionally modelled using different sets of equations describing heat and mass transfer for successive stages of drying, separated by pre-defined end conditions. By incorporating the mechanical behaviour of the particulate phase with appropriate evolution laws, we solve a single set of governing equations. Different granule microstructures are obtained (e.g. dense granule, loose granule, hollow shell, expanded hollow shell, etc.) depending on the evolving strength and permeability of the granular skeleton, evaporation rate, heat and mass transfer rates withing the droplet and with the surrounding atmosphere.
2. Swelling and disintegration of multi-component polymeric structures is modelled considering mass transfer and transformations in the solid phase. By incorporating the mechanical response (through a swelling stress) and material properties such as elastic parameters and failure models which evolve with fluid ingress, it is possible to describe 1) drug release profiles for controlled release tablets or 2) breakup of immediate release tablets. Similar to droplet drying, the behaviour can be modelled using a single set of governing equations with suitable parameter evolution laws.
3. Fungi growth on grain storage silos has significant quality, safety and economic implications. Fungi growth is modelled using a rate equation which can incorporate moisture content, temperature, oxygen content, and other parameters. For example, fungi growth rate is affected by temperature, which is determined by solving heat transfer equations, considering silo size and outside temperature fluctuations during day/night or over longer timescales, as well as the metabolic heat generation due to fungi growth. Relative humidity depends on the temperature of the air and moisture migration is described by diffusion. The local oxygen content is also described using diffusion. The mechanical contact areas between two individual grains arising due to self weight affects and is affected by the heat and mass transfer processes.

The application examples discussed above demonstrated that coupling mechanical behaviour with chemical reactions and heat and mass transfer offers a unified framework that provides greater insight and enables more accurate modelling for better material and process design. While solving coupled equations no longer presents technical difficulties, the experimental data requirements for model calibration have increased.

Acknowledgement: I’d like to acknowledge former PhD students Abdulrahman Ramahi and Amnani Binti Shamjuddin and current PhD student Badran Salim who researched the three topics above, respectively.

Lectures: Riešenia pre energetickú transformáciu priemyslu - SK session

Linda - Vývoj a implementácia lean digitálnej prevádzkovej dokumentácie pre vybrané energetické prevádzky v závode Volkswagen Slovakia

Juan Chávez-Fuentes

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Key words: Lean digitalizácia, agilita, prevádzková dokumentácia

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Abstrakt

Tepelné čerpadlá: Dekarbonizácia a efektívne využitie odpadového tepla

Autor: Ing. Michal Jurovich, Volkswagen Slovakia, a.s.

Prednáška sa zameriava na inovatívne riešenie vykurovania v závode Volkswagen Slovakia, a.s., ktorého cieľom je znížiť uhlíkovú stopu a zároveň efektívne využiť existujúce zdroje odpadného tepla. V úvode bude predstavený aktuálny stav horúcovodného systému v závode a centrálneho zdroja tepla, ktorý slúži prioritne na zásobovanie technologickým teplom a teplom na vykurovanie výrobných hál a taktiež administratívnych objektov. Následne bude popísaný proces integrácie priemyselných tepelných čerpadiel do vykurovacieho systému výrobných hál, s dôrazom na technické aspekty a výzvy spojené s implementáciou. Tretia časť prednášky sa bude venovať prevádzkovaniu a regulovaniu tepelných čerpadiel v synergii s existujúcou centrálnou výhrevňou**,** vysvetľujúc stratégiu riadenia pre optimálnu efektivitu a spoľahlivosť systému. V závere bude prezentovaná rentabilita nasadených riešení, úspor energie a očakávanej návratnosti investície.

Posters

Posters: Bioprocess and biotechnology

Antibiotic Efficacy Against *Pseudomonas aeruginosa* Biofilms: Synergistic Role of Allicin in Chronic Respiratory Infections

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Keywords: biofilm formation, allicin, antimicrobial synergy, pulmonary environment

Infections associated with bacterial biofilm formation caused by *Pseudomonas aeruginosa* present a therapeutic challenge, particularly in patients suffering from chronic respiratory conditions like cystic fibrosis. Biofilms promote the survival of bacterial populations by limiting the penetration and efficacy of antimicrobials, which contributes to increased resistance and complicates eradication. This tolerance allows the pathogen to persist at sites of infection despite ongoing treatment. As resistance to conventional antibiotics increases, there is a growing demand for combination strategies that can improve treatment outcomes and reduce the selective pressure for resistance development. Allicin, a natural compound derived from garlic, has demonstrated antimicrobial properties and the potential to enhance the activity of antibiotics. In this study, we investigate the effect of allicin in combination with selected antibiotics, namely kanamycin and polymyxin B, on inhibiting *P. aeruginosa* biofilm formation. The antimicrobial efficacy of individual and combined treatments was evaluated by monitoring bacterial growth dynamics and assessing biofilm viability after treatment using standard colorimetric and kinetic assays. This approach enabled observation of not only the overall antimicrobial effect but also potential synergistic interactions between tested compounds. Alongside standard *in vitro* conditions, preliminary experiments included structural modifications designed to approximate characteristics of the pulmonary environment, such as increased viscosity. These elements were incorporated to explore whether more physiologically relevant conditions might influence treatment outcomes. Although this aspect of the study is still being developed, it represents a significant step toward a better understanding of therapeutic performance in environments that mimic chronic lung infections.

Acknowledgements:
This research has been supported by the Ministry of Education, Youth and Sports of the Czech Republic grant Talking microbes - understanding microbial interactions within One Health framework (CZ.02.01.01/00/22_008/00045) and by the Czech Science Foundation (GAČR), project No. 23-07356S.

Binding of Polyclonal Antibodies on a Multimodal Membrane Adsorbents

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Key words: multimodal adsorbents, membrane adsorbents, proteins, chromatography

Antibodies play a crucial role in the treatment of various diseases, including asthma, cancer, autoimmune disorders, and transplant rejection. With advancements in recombinant technology, the ability to produce high titers of antibodies in culture media has significantly increased. However, this increase in product concentration has led to higher demands in downstream processing. It is estimated that an increase in the product concentration to 10 g L^{-1} increases the specific costs downstream from 61 to 97 %.

The common separation section contains several chromatographic steps supplemented by multiple additional devices such as filters or desalination modules. One potential solution to reduce the complexity and cost of this process is the use of multimodal membrane adsorbents. Unlike conventional chromatographic adsorbents, these resins provide more than one type of interaction with the target protein. Another advantage of membranes compared to beads is lower pressure loss, lower mass transfer resistance, and higher flow rates. These are the advantages that allow such adsorbents to process large volumes of media.

In this study, we evaluated three prototype membrane adsorbents with varying agarose content for their binding capacities to polyclonal antibodies and bovine serum albumin (BSA). We first measured the ligand density for each membrane. The highest ligand density, 104 mmol mL^{-1}, was measured for the membrane with the highest agarose content. In contrast, the membrane with the least agarose has a ligand density of approximately 77 mmol mL^{-1}.

The second step in our work was devoted to the measurement of static binding capacities (SBC) of membrane adsorbents. For polyclonal antibodies, the SBC ranged from 9.7 to 11.7 mg mL^{-1}, with the highest value observed in the membrane with the highest ligand density. In contrast, for BSA, significantly higher binding capacities were observed. They range from 50 to over 80 mg mL^{-1}, with increasing ligand densities.

Finally, we tested membranes under dynamic conditions using antibodies. Although the binding capacities were lower in the dynamic conditions, we were able to separate the monomeric form of protein from its aggregates.

Acknowledgements: This work was supported by grants from the Slovak Research and Development Agency (Grant number: APVV-20-0312) and Scientific Grant Agency of the Slovak Republic Grant number: VEGA 1/0515/23.

Biodegradation of Ibuprofen Salt in SBR Reactor with Activated Sludge under Aerobic Conditions

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Key words: pharmaceuticals in wastewater; biological treatment; bioreactor SBR; ibuprofen salt; biodegradation

In recent decades, there has been a marked increase in the concentration of pharmaceuticals in wastewater, a direct result of their increasing availability and widespread use in the society. One of the most commonly detected substances is ibuprofen (IBF), a widely used nonsteroidal anti-inflammatory drug (NSAID) commonly used as a painkiller.

The present study analyzed the biodegradation process of a selected pharmaceutical over time. The study was conducted for three different concentrations of ibuprofen salt in the feed stream: 4, 10 and 20 mg IBF/L. The SBR cycle consisted of filling, aeration, settling and drawing phases. In addition, an adsorption test was performed using activated sludge inactivated with sodium azide – in order to assume the contribution this physico-chemical process to the overall removal efficiency of the bioreactor. The samples were analyzed using liquid chromatography (Nexera LC-2040C 3D Plus, Shimadzu, Kinetex column C18 100x3mm). The results showed the high efficiency of IBF stream treatment by biological methods. During one cycle, up to 90% (maximum 18 mg IBF/L) of the introduced NSAID was removed. The adsorption test revealed that maximum 2 mg IBF/L could be removed by adsorption on activated sludge. The samples were also analyzed for the potential products of ibuprofen metabolism, such as: 1-hydroxyibuprofen, 1-[4-(2-methylisopropyl)phenyl]ethan-1-ol, 4-ethylbenzaldehyde and ethyl-4-ethoxybenzoate. Although, probes were taken every 30 minutes during the aeration phase, none of the products were detected. The most likely explanation is that the above mentioned intermediates were rapidly metalobized to smaller products. This study, demonstrated that the process in the SBR type reactor is an effective method for IBF removal in which the biodegradation is the dominant mechanism responsible for the removal of the pharmaceutical.

Acknowledgement: Financial support from the National Science Centre (Poland) under project number 2021/43/B/ST8/001854 is acknowledged.

Dark fermentation of liquid after hydrothermal treatment of kitchen waste

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Key words: dark fermentation, hydrogen, thermal pretreatment, kitchen waste, green energy

Dark fermentation (DF) is a promising biological process for the conversion of wet organic waste into hydrogen-rich gas. This study investigates the potential of liquid fractions derived from thermally pretreated kitchen waste as substrates for DF. Two thermal pretreatment strategies – thermal hydrolysis and hydrothermal carbonization – were applied over a wide temperature range, with a fixed treatment time. For one specific temperature, an extended treatment time was also tested to evaluate the impact of prolonged hydrolysis.

Fermentation experiments were conducted under mesophilic conditions using inoculum sourced from fermented sludge (Group Wastewater Treatment Plant in Lodz), heat-treated at 70°C to suppress methanogenic activity. Process performance was evaluated through hydrogen production yield (mL H_2/g_{TVSKW}), pH and dissolved organic carbon (DOC) pre- and post-fermentation, and also by volatile fatty acid (VFA) composition after fermentation.

The results clearly show that pretreatment temperature has a significant effect on the efficiency of hydrogen production. Certain conditions resulted in significantly higher yields, while both insufficient and excessive pretreatment hindered the process. In one case, extending the treatment time significantly improved substrate availability, resulting in enhanced hydrogen production.

Overall, the results emphasize the importance of optimizing thermal pretreatment parameters. When properly adjusted, thermal pretreatment can effectively balance substrate solubilization with the preservation of hydrogen-producing microbial activity. Conversely, non-optimal conditions can severely limit DF performance, probably due to incomplete hydrolysis or the formation of inhibitory compounds.

Acknowledgement

This research was funded by the National Science Centre (2021/43/B/ST8/00298).

Enhanced taxanes production by *Taxus x media* hairy roots in cultures supported with hybrid silica-chitosan aerogel-based materials

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Key words: chitosan-modified silica aerogels, taxanes, transgenic roots, *in vitro* cultures, plant biomass, metabolism stimulation

Taxanes,, i.e., paclitaxel or docetaxel, are essential drugs in modern oncology. They are frontline chemotherapeutic agents for breast, ovarian, and lung cancers, and they are also used in prostate cancer and Kaposi's sarcoma. Despite their clinical success, the widespread application of taxanes is limited by a lack of natural sources or production systems. The low yield of paclitaxel production from natural sources, and the increasing global demand emphasize the necessity for innovative strategies for taxanes production. Given the metabolic complexity and low yields in natural sources, efforts to taxane biosynthesis in microbial systems, plant biomass *in vitro* bioprocessing, or cell-free platforms are recognized as crucial solutions for the efficient production of paclitaxel. Furthermore, the versatility of *in vitro* culture systems creates the possibility for enhanced metabolite production by the application of the bioengineering method. The use of hybrid chitosan-modified silica aerogels allows for simultaneous immobilization of the plant biomass and its directed elicitation, which can allow to overcome actual problems with plant-origin paclitaxel production.

The aim of the study was to investigate the influence of two various aerogels containing methyl (TMCS) and hydroxyl (TEOS) groups, and their combinations with chitosan, on *Taxus x media* transgenic roots biomass proliferation and taxanes production. Plant biomass was cultured with TMCS and TMCS-chitosan or TEOS and TEOS-chitosan aerogels. For hybrid chitosan-silica aerogels, the following concentration of chitosan for 1g of aerogel: 0.05g, 0.1g, 0.2g, and 0.4g, has been noted. The increase in the amount of plant biomass and biosynthesized taxanes was determined quantitatively.

The application of TEOS and TMCS aerogels has a slight effect on plant biomass growth and shows a noticeable influence on the production of taxanes. Supporting culture systems with chitosan-modified silica aerogel caused an increment in the production of secondary metabolites. The increase in chitosan concentration in aerogel improved the taxane concentration.

Acknowledgments

This work has been funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program (YOUNG PW II).

Enhancing ε-Caprolactone Production via a Multienzyme Cascade in E. coli: Impact of Oxygen Transfer and Ethanol as a Competitive Inhibitor

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Key words: ε-Caprolactone, Baeyer-Villiger oxidation, enzyme cascade

ε-Caprolactone is an important monomer in the industry, which can be polymerized into polycaprolactone. Traditional chemical synthesis of lactones uses Baeyer-Villiger oxidation (BVO) of ketones using peracids, which has disadvantages such as low selectivity and formation of harmful by-products. In this study, we present a sustainable alternative via whole-cell biocatalysis using a three-enzyme cascade (ADH, ER, CHMO) that efficiently converts 2-cyclohexanone-1-ol to ε-caprolactone.

We investigated the effect of oxygen transfer coefficient (kLa) and substrate concentration (cs) on the efficiency of oxidation of cyclohexanone to ε-caprolactone. The results indicate a strong dependence of the cascade rate on the correct ratio between kLa and cs, due to the simultaneous metabolic consumption of oxygen by the cells themselves.

We further studied the effect of ethanol as an inhibitor of ADH, which catalyzes not only the first step of the cascade but also the reaction of cyclohexanone to the undesired by-product cyclohexanol. Our study showed that there is an optimal concentration of ethanol that inhibits the side reaction without significantly suppressing the desired ADH activity. These results contribute to a better understanding of kinetic interactions within multi-enzymatic reaction networks and provide a basis for the design of more efficient biocatalytic processes.

Acknowledgment: This work was supported by grants from the Slovak Research and Development Agency (Grant number: APVV-20-0272) and the Scientific Grant Agency of the Slovak Republic (Grant number: VEGA 1/0515).

Flow Chemistry for the Enantioselective Synthesis of Chiral Cyanohydrins

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Key words: chiral cyanohydrins, flow chemistry, Henry reaction, heterogeneous biocatalysts, hydroxynitrile lyases, silica carriers

The demand for chiral cyanohydrins has been steadily increasing due to their broad applications in various industries, such as horticulture, cosmetics, pharmaceuticals, and, notably, the chemical industry. These compounds serve as valuable intermediates in the synthesis of *fine chemicals*, including α-hydroxy acids, aldehydes, ketones, and amines. Despite their importance, the chemical synthesis of chiral cyanohydrins often involves complex procedures, prompting the exploration of biocatalytic routes as a more sustainable alternative.

Flow chemistry has emerged as a powerful approach in chemical synthesis, providing precise control over reaction conditions and enhancing scalability compared to traditional batch processes. This continuous mode facilitates efficient heat and mass transfer, making it promising for reactions involving complex biocatalysts. The combination of flow chemistry with biocatalysis not only improves reaction efficiency but also reduces waste and energy consumption, aligning with *green chemistry* principles. In this context, the Henry reaction, involving the addition of a nitroalkane to a carbonyl compound, is particularly relevant for synthesising chiral cyanohydrins, producing valuable intermediates like β-nitroalcohols.

In this study, we investigated the covalent immobilisation of hydroxynitrile lyase from *Granulicella tundricola* (*Gt*HNL-3V) on organically modified monolithic microreactors (MHs) with amino (A) and octyl (O) groups. The activity, stability, and enantioselectivity of the heterogeneous biocatalysts were evaluated in the continuous synthesis of chiral cyanohydrins: *R*-mandelonitrile in an organic medium with buffer saturation and *R*-1-phenyl-2-nitroethanol in a biphasic system.

Acknowledgement: The corresponding author gratefully acknowledges the general financial support from the Ministry of Science and Higher Education (Poland) program under grant PERŁY NAUKI agreement PN/01/0267/2022.

How can we study tuberculosis using microfluidic chip?

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Key words: microfluidics, tuberculosis, *Mycobacterium Smegmatis*

Tuberculosis (TB) is a highly infectious disease that continues to affect 10 million people worldwide, resulting in over a million deaths each year. This is despite the high availability of the BCG vaccine and various antibiotics and largely due to rising antibiotic resistance. Traditional methods of TB research are complicated by the need for biosafety level 3 (BSL-3) facilities for handling *Mycobacterium Tuberculosis* (MTB). Using the non-pathogenic *Mycobacterium smegmatis* (MSMG) as a model organism leverages its physiological and metabolic similarities to MTB while providing a safer and more accessible alternative for studies in BSL-1 laboratories.

A key approach in advancing TB research involves the use of microfluidic chips, which enables precise control over experimental conditions at a microscale, leading to reduced sample consumption while improving experimental reproducibility. These devices enable monitoring of bacterial morphology, growth patterns, and responses to environmental stressors, such as oxygen depletion and antibiotic exposure by mimicking the conditions mycobacteria encounter in the human body.

The design and fabrication of microfluidic devices involve soft lithography techniques, where PDMS is moulded onto a master wafer. The PDMS structure is then bonded to a glass slide using oxygen plasma treatment, creating a sealed microchannel network. The fabrication process ensures reliable bacterial trapping, nutrient supply, and optimal conditions for live-cell imaging. The aim of this work is to integrate MSMG with optimized microfluidic chips to contribute to more efficient TB studies by mimicking *in vivo* conditions and through improved visualization and real-time monitoring of bacterial behaviour. This approach has the potential to lead to better diagnostics and therapeutic interventions.

Intensified naphthoquinone biosynthesis in *Rindera greaca* transgenic roots cultured with hybrid PLA-chitosan scaffolds

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Keywords: transgenic roots, secondary metabolites, *Rindera graeca*, elicitation, biomaterials

Plants show great potential as a source of biochemical compounds worldwide. They are characterized by high biodiversity, which offers potentially enormous quantities of biologically active substances with a wide spectrum of applications in the pharmaceutical industry. The usage of in vitro methods for plant biomass culturing enhances the productivity of secondary metabolites in comparison to wild plants. Moreover, specific bioengineering techniques can be used to improve biomass proliferation and the desired metabolite biosynthesis. The hybrid polymer–elicitor scaffolds can be a promising tool to increase the production of secondary metabolites, due to the simultaneous utilization of plant biomass immobilization and elicitation. The study aimed to investigate the impact of chitosan characteristics on the naphthoquinone biosynthesis and biomass proliferation of *Rindera graeca* transgenic roots.

The hairy roots were placed on the top of hybrid scaffolds made of polylactic acid (PLA) blended with chitosan to conduct the cultures. The elicitor used in this study was squid and fungi origin. In the case of fungal chitosan, three chitosan molecule masses, i.e., 30 kDa, 300 kDa, and 3000 kDa, and different viscosities, i.e., 10-120 cps, 100-300 cps, and 2000-3500 cps, were used. The average concentration of the polysaccharide obtained in the used constructs was around $25\%_{m/m}$. Transgenic roots immobilized on PLA scaffolds without chitosan were used as a control system. The growth of the biomass and the produced naphthoquinones in *Rindera graeca* transgenic root cultures were determined quantitatively.

The squid chitosan causes intensified hairy root proliferation compared to the fungal chitosan and the control system. However, the biomass cultures with fungal chitosan produced significantly more naphthoquinones than cultures containing polymeric scaffolds modified with squid chitosan. Along with the increase in the mass of the chitosan molecule, the increase in the plant biomass was noticed. The highest naphthoquinone concentration was noticed for scaffolds containing 300 kDa chitosan. The chitosan viscosity had no notable effect on biomass proliferation and the production of naphthoquinones.

Acknowledgments
This work has been funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program (Mobility PW).

Optimization of reaction parameters by factorial design for the enzymatic synthesis of natural aroma esters

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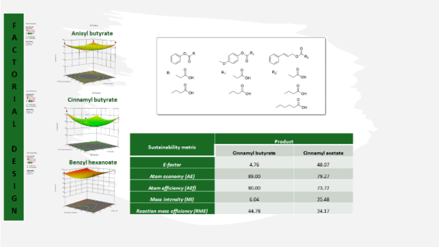
Key words: aroma ester; factorial design; lipase; sol-gel; green chemistry

In recent years an increase in the public's demand for bio-products has been observed. This has prompted increased efforts by the food and agricultural industries to develop alternative methods for preparing food ingredients with significantly reduced environmental impact in order to satisfy the general public's needs.

The current work shows the synthesis of seven aroma esters (anisyl propionate and butyrate, cinnamyl propionate and butyrate, benzyl propionate, butyrate and hexanoate) by direct esterification of carboxylic acids with the corresponding alcohols mediated by lipase B from *Candida antarctica* encapsulated in a sol-gel matrix in a solvent-free system using vacuum to remove the resultant water. The reaction parameters were optimized for each reaction system by factorial design experiments considering four factors (acid excess, temperature, applied vacuum and reaction time) on two levels. This study presents an alternative to the currently applied method for obtaining aroma esters which is extraction from natural sources.



Sustainability metric	Product	
	Cinnamyl butyrate	Cinnamyl acetate
E-factor	4.76	48.07
Atom economy (AE)	89.00	79.27
Atom efficiency (AEf)	80.00	73.72
Mass intensity (MI)	6.04	35.48
Reaction mass efficiency (RME)	44.78	34.17

By applying factorial design method (central composite) for optimization of each reaction the conversions were significantly increased (for example, from an isolation yield of 49.4% to 94.3% for cinnamyl butyrate). A semi-preparative experiment was further set-up for cinnamyl butyrate preparation and green chemistry metrics were determined for the above-mentioned synthesis. A mass intensity of 6.04 and a *E*-factor of 4.76 demonstrated that the newly developed enzymatic process is suitable for industrial application based on the green chemistry principles.

Acknowledgements

Financial support for this work was received through the project Advanced (multi)-enzymatic synthesis and purification processes for bio-based furan derivatives – ASPIRE, project code CF 25/14.11.2022, 2023-2026.

Purification of post fermentation broths applying microalgae

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Key words: biohydrogen; algae; dark fermentation; photofermentation; biorefining

Microalgae offer a promising solution by absorbing nutrients, reducing eutrophication, and sequestering carbon dioxide. This approach is energy-efficient and sustainable, with the added benefit of producing biomass that can be used for biofuels and other products. Microalgae can also remove pathogens and heavy metals, improving water quality. The research involves the application of microalgae from the Baltic Sea, a region with significant pollution, to develop a purification process. This research is crucial due to ecological changes in the Baltic ecosystem. Algal biological processes, particularly direct biophotolysis, involve the photosynthetic production of hydrogen from water. Algae like *Chlamydomonas reinhardtii, Platymonas subcordiformis,* and *Chlorella species* are efficient at capturing solar energy and producing hydrogen. Increasing cell density and adding external carbon sources like sugars can enhance hydrogen production. Creating anaerobic conditions is crucial for algae to switch from oxygen to hydrogen production. The research proposes using microalgae to detoxify fermentation broths and biofiltration effluents. It focuses on bioenergy and bioprocesses as sustainable energy solutions, crucial for transitioning to a low-carbon future and aims to establish effective biological cleaning systems and strategies for managing leachates and post-fermentation broths. The scientific novelty lies in using model and natural-origin microalgae to develop a sustainable method for purifying sewage streams, optimizing growth conditions, and contributing to a circular economy. Untreated sewage introduces harmful pollutants into aquatic ecosystems, posing health risks to humans and wildlife, and causing eutrophication, which depletes oxygen levels and harms aquatic life. Aging sewage infrastructure exacerbates these issues by causing frequent overflows and leaks. Effluents from fermentation and biofiltration have varying compositions and environmental impacts. Fermentation effluents have high organic matter, leading to elevated biochemical and chemical oxygen demand. Biofiltration reduces organic pollutants but may leave residual nutrients. Comprehensive treatment of all effluents is essential to minimize environmental impact and ensure regulatory compliance

Funding: The research was financed by National Science Centre throughout project: UMO-2021/41/B/ST8/02395 from 2021-11-26 “Management of bio fraction waste for two-stage biohydrogen production with simultaneous treatment of gaseous streams with green solvents”.

Testing the Biodegradation of Diclofenac: Towards a Sustainable Environment

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Key words: pharmaceuticals in wastewater; biological treatment; bioreactor SBR; diclofenac;

The presence of pharmaceuticals in wastewater is becoming an increasingly serious threat to the aquatic environment and public health. Pharmaceuticals are typically, used in small therapeutic doses, but often enter wastewater systems. Mainly through excretion from the body, but also as a result of inadequate disposal of outdated medicines. The increased availability of medicines and the public's tendency to misuse them exacerbate the problem. In addition, many pharmaceuticals are not completely removed by conventional wastewater treatment systems, leading to their accumulation in the aquatic environment with a range of consequences for the receiving ecosystem. One particular medicine, is diclofenac (DFC) - an anti-inflammatory drug. Due to its toxic effects on aquatic organisms, its presence in the environment needs be monitored and its discharge into surface waters needs be restricted. The introduction of DFC into the environment can lead to many other negative effects. Its presence in wastewater and water is therefore a serious challenge for modern environmental engineering, requiring the development of effective methods and technologies to prevent its introduction into the environment.

In the present study, an attempt was made to biodegrade diclofenac using SBR-type bioreactors – working in the cycles consisting of the filling aeration, settling and drawing phases. Firstly, the adsorption of DFC on activated sludge was tested – after the inactivation by sodium azide. After 60 minutes of the experiment, a 20% reduction in DFC content on the activated sludge was recorded. DFC biodegradation studies were conducted for 3 different concentrations: 4, 10 and 20 mg DFC/L. During the experiment, no effective removal of diclofenac from the introduced model wastewater stream was observed. On the contrary, a gradual accumulation of the selected drug was observed in the bioreactor, which may indicate its stability under the conditions of the applied process and its overall limited biodegradability.

Acknowledgement: Financial support from the National Science Centre (Poland) under project number 2021/43/B/ST8/001854 is acknowledged.

The application of β-D- galactosidase from *Bifidobacterium bifidum* in the synthesis of galactooligosaccharides

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Key words: deep eutectic solvents, galactooligosaccharides, galactosidase, hydrolysis, transgalactosylation

Galactooligosaccharides (GOS) are a class of functional oligosaccharides considered prebiotic. GOS selectively stimulate the growth of beneficial bifidobacteria in the gut, contributing to improved gut health and overall well-being. GOS have been shown to increase probiotic viability and antioxidant activity in fermented products.

The aim of the experiments was to evaluate the preference of β-D-galactosidase from *Bifidobacterium bifidum* in the galactooligosaccharide synthesis reaction. Reactions were carried out in aqueous solutions of lactose and in the environment of deep eutectic liquids (DES). The composition of the reaction mixture was analyzed using liquid chromatography with refractometer and scattered light detector. Favorable synthesis of GOS (about 30%) was found in the reaction catalyzed by NURICA in 20-40% of lactose solutions and at 40-60°C.

At temperatures up to 30°C, the transgalactosylation reaction occurred slowly and less efficiently. During transgalactosylation reactions carried out at 70 and 80°C, the enzyme is inactivated.

In the reaction catalyzed by NURICA in a deeply eutectic liquid medium (choline chloride:glucose, 1:2 M), preferential catalysis of the hydrolysis reaction was observed.

Project funded under the designated subsidy of the Minister of Science and Higher Education Republic of Poland, task entitled: The Research Network of Life Sciences Universities for the Development of the Polish Dairy Industry – Research Project.

The effect of phytoextracts obtained from *Cistus incanus* on the growth of lactic acid bacteria

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Key words: *Cistus incanus,* phytoextracts*, Lactobacillus acidophilus, Lactobacillus sanfranciscensis*

Phytoextracts represent a rich source of bioactive compounds, including polyphenols. Plant extracts are characterized by notable antioxidant and antimicrobial properties. Polyphenols can effectively inhibit undesirable transformations in food, thereby extending its freshness. At appropriate concentrations, phytoextracts may also support the growth and viability of lactic acid bacteria. These bacteria can facilitate the fermentation of polyphenols, enhancing their bioavailability, generating novel intermediates, and increasing the total polyphenol content.

The aim of this study was to assess the impact of phytoextracts from Turkish rockrose (*Cistus incanus*), obtained via maceration using aqueous methanol solutions, on the growth and development of selected strains of lactic acid bacteria: *Lactobacillus acidophilus* 5e2, *Lb. sanfranciscensis* DSM20663, and *Lb. sanfranciscensis* DSM20451. The extraction yield was evaluated depending on the solvent used, and the concentration of polyphenols and their antioxidant activity in the extracts were determined. The highest extraction yield was observed for the sample extracted with water (15.48 ± 0.27%), while the lowest yield was recorded for the sample macerated with 99.8% methanol (7.72 ± 0.08%). Extracts obtained from *Cistus incanus* using a 50% aqueous methanol mixture contained the highest polyphenol content (0.93 mg/cm^3). The strongest antioxidant activity was exhibited by extracts obtained with both water and 99.8% methanol. The addition of *Cistus* extracts to the culture medium at concentrations ranging from 0.5% to 1% inhibited the growth of the studied bacterial strains. In contrast, the addition of *Cistus* extract in the concentration range of 0.005% to 0.1% stimulated the growth of *Lb. sanfranciscensis* DSM20663 and *Lb. sanfranciscensis* DSM20451.

Valorization of Charry Pit Waste: Efficient Oil Extraction for Biodiesel Production

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Key words: Waste oil, Biodiesel feedstock, Stone fruit waste, *Oblačinska* variety (*Prunus cerasus L.*), Solvent extraction

Making chemicals and biofuels from biomass is one of the most promising approaches. Growing concerns over land and water use, deforestation and food security have challenged the sustainability of traditional biodiesel feedstocks. Waste from stone fruit, such as cherry seeds, offers a promising, low-cost, and low-acid feedstock for biodiesel production due to its high-oil content (above 50% of seed mass), and the large amounts of waste generated by the food industry, posing significant environmental challenges. This study presents preliminary results of oil extraction from cherry pits of the *Oblačinska* variety (*Prunus cerasus L.*), as a potential step toward their valorization in second-generation biodiesel synthesis.

In order to achieve optimal yield and oil quality, solvent extraction was performed on both finely milled whole kernels (shall + seed) and separated seeds, using several non-polar solvents, with or without the use of a Soxhlet apparatus. The effect of extraction time on oil yield was initially tested. Interestingly, the results revealed no significant increase in oil yield beyond 5 min, ranging from 26,9±1,1% to 28,4±0,42% for seeds, while similar trends were observed in previous extractions from whole cherry pits. These findings suggest that nearly complete oil extraction can be achieved within five minutes, highlighting the efficiency of the process for potential upscaling. The short extraction time is attributed to the high oil accessibility in cherry seeds, fine particle size, and the use of petroleum ether as an effective non-polar solvent.Detailed analysis of the extracted oils included acylglycerols, phospholipids, hydrocarbons, and pigments, using GC-MS, GPC, HPLC, HPLC-MS, and Raman spectroscopy. Fatty acid profiling was conducted by GC–MS/FID after derivatization.

Acknowledgements: This research was supported by the European Project 101179991- VERDEDRIVE - HORIZON-MSCA-2023-SE-01 titled: "Harnessing by-products for the creation of eco-friendly and sustainable diesel fuel".

Posters: Risk management and process safety

Analysis of chemical process response to the deviation of multiple input parameters

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Key words: nonlinear system; hazard identification

Modern chemical industry uses more sophisticated units and equipment. These units allow us to produce complex products with less emissions emitting and more effective energy consumption. However, using more complex units creates challenges in design, control, analysis, process safety, and economics. Chemical processes behavior is naturally nonlinear, and this behavior is mainly shown during malfunctions. The behavior of complex units is harder to predict and can hide more nonlinearities in process out parameters. Nonlinear behavior can be detected in small or wide working range of input parameters, in some cases, it can appear due to specific combinations of input parameters. Nonlinear response can occur in other pieces of equipment of unit than where input parameter deviation appears. Dangerous behavior created by combination of independent input parameters can be overlooked during hazard analysis, e.g. HAZOP. The nonlinear system response can be detected as oscillatory behavior, domino effects or high sensitivity to change in input parameters (fast change in temperature, pressure or runaway effect). Identification of nonlinear behavior can be applied to the unit with input parameter deviation from design value, but it can be applied also to connected units and equipment. Analysis of the unit with deviation and connected units can find domino effects, nonlinear response only at connected unit etc. Usage of mathematical modeling supported hazard analysis can detect more potentially dangerous scenarios, which are hardly predictable because of complex units and processes.

System response to multi-input parameter deviations is analyzed via Morris sensitivity analysis (1991). This methos is used to analyze defined range of possible deviation values. It uses one-at-time sampling method for analysis. Results of Morris analysis are parameter influence on system response and nonlinear effect and/or interactions with other analyzed inputs. Analysis is performed on propylene glycol production case study. Aspen Plus Dynamics® was used as a simulation tool for the chemical plant and Matlab® was used to evaluate Morris method. The analysis was performed in two modes: durations of deviations were shorter than one hour and infinity duration of deviations. Deviated input parameters were propylene oxide flow, water flow, cooling water flow and temperature of cooling water. The chemical plant consists of the continued stirred tank reactor and two columns. Analyzed output parameters are reactor temperature, condenser temperature of both columns and reboiler temperature of both columns. Water flow has the strongest influence on system response and nonlinear effect. Analysis including deviation duration shows also strong influence of duration of water flow deviation but decrease influence of propylene oxide flow deviation.

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CFD-assisted experimental analysis and optimization of air quality in production space

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Key words: HVAC, Computational Fluid Dynamics (CFD), air quality management

Air quality management plays a vital role in ensuring process and workplace safety. Consequently, an effective heating, ventilation, and air-conditioning (HVAC) system is essential for contemporary production operations. This is particularly critical in the pharmaceutical sector, where there is a significantly greater risk of hazardous product contamination or worker exposure.

Computational fluid dynamics (CFD) modeling has become an integral component of the HVAC system design and evaluation process. While parameters specified during HVAC design, such as volumetric flow rates, are typically straightforward to obtain, actual working conditions can significantly deviate from these values, particularly in older HVAC systems. To address this, a two-step experimental model validation approach is employed to ensure that the model accurately reflects the current state of the HVAC system. Hot-wire anemometry is primarily utilized to measure true velocity boundary conditions at the points where air enters or exits the area of interest. Additionally, a local tracer gas (CO_2) source is implemented to assess flow and mixing conditions within the areas where the flow direction may not be constant or well defined.

OpenFOAM is utilized to develop a CFD model of the actual production space. This model employs a RANS density-based solver and incorporates ideal gas thermodynamics for air mixture. This configuration enables the model to effectively capture high concentrations of CO_2 as well as the spatio-temporal distribution of composition and temperature. Once validated, the CFD model can be employed to analyze specific airflow characteristics produced by the HVAC system and their impact on effective air quality control. The mean age of air (MAOA) is selected as an indicator of air quality, while the overall volumetric flow rate serves as a measure of energy costs. The relationship between the parameters of the HVAC system and MAOA was thoroughly examined.

Numerical method of testing the flow parameters of positive pressure ventilators on the ISO 5801 test stand

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Key words: positive pressure ventilators, airflow, iso 5801, CFD, LES

Positive pressure ventilators are an important tool used in rescue operations by fire protection units. The aim of this article is to assess the potential of using LES-type analyses for CFD simulations (in the Fire Dynamics Simulator software) to evaluate the flow parameters of a positive pressure ventilator under the conditions of the PN-EN ISO 5801 method. The article presents a comparative analysis that enables an assessment of the level of convergence between the volumetric airflow rate and pressure obtained in full-scale experimental studies and numerical CFD analysis. For the airflow rate [m³/h], a convergence of 1.4% was achieved, while for pressure [Pa], the convergence was 17%. The analysis demonstrated that the LES model is an appropriate tool for reflecting the conditions specified by the PN-EN ISO 5801 method. The CFD simulation method described in the publication may serve as a useful tool for manufacturers of positive pressure ventilators, enabling the implementation of technological pre-tests without the need for costly laboratory experiments.

Posters: Environmental chemical engineering

Advanced methods for the assessment of waste elastomer fillers

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Key words: waste elastomer, oscillatory rheology, mechanical recycling, inverse gas chromatography, calorimetry, SEM

In this study, the incorporation of waste elastomers, including ground tire rubber (GTR) and ethylene propylene diene monomer (EPDM) rubber into a waste high-density polyethylene (w-HDPE) matrix was investigated, with the focus on the impact of particle size and homogenization time on the mechanical, rheological, and structural properties of the resulting blends. The elastomeric fillers were fractionated into different particle sizes, and their interactions with the polymer matrix were analyzed using mechanical testing, oscillatory rheometry, scanning electron microscopy (SEM), calorimetry and inverse gas chromatography (iGC). It was found that the mechanical properties, particularly impact strength and elongation at break were significantly influenced by the particle size distribution and the homogenization time. Smaller elastomer particles enhanced the interface area, improving stress transfer and extending the linear viscoelastic (LVE) range, but excessive fractionation led to agglomeration, which diminished the mechanical properties. Rheological analysis revealed a relationship between the crossover frequency and the dispersion of elastomer particles, with the blend containing the smallest particle size exhibiting the highest molecular weight but poor homogeneity due to agglomeration. SEM images further confirmed the tendency for particle aggregation in blends with the smallest elastomer fractions. The results suggest that particle size distribution and sufficient homogenization time are critical for optimizing the dispersion of elastomer fillers in polymer matrices. Practical recommendations include the use of frequency sweep tests to assess whether fractionating elastomer fillers into specific size ranges would be beneficial for improving blend properties.

Green and white method for the determination of selected essential and toxic elements in vegetable and meat-based samples by small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry and combustion-assisted digestion

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Key words: microplasma source, essential element, toxic element, combustion-assisted digestion

The determination of essential and toxic elements, such as Se, Zn, Cu, Cd, Hg and As, using green sample preparation techniques coupled with miniaturized instrumentation, is a critical research focus in the field of analytical methods development. Thus, the aim of this study was the development of a green and white method based on oxygen flask combustion of the sample, and detection by optical emission spectrometry using small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry. The microsample (10 µL) was vaporized from a small-sized Rh-coiled filament, while the low power (15 W) and low Ar consumption (150 mL min^{-1}) microplasma was used as excitation source and a low-resolution microspectrometer was used for recording the multielemental spectrum. The combustion method, as a greener alternative to wet acid digestion, involved weighing 50–100 mg sample, wrapping it in a small ashless filter paper, and placing it in a platinum basket. The sample was then combusted in an oxygen-filled Erlenmeyer flask, and the combustion gas was absorbed in a volume of 10 mL 0.1 mol L^{-1} HCl solution. In order to verify the effectiveness of the combustion-based digestion, the samples were microwave-assisted digested in concentrated HNO_3 - H_2O_2 mixture. The accuracy (recovery and precision) of the method was evaluated by analyzing several certified reference materials (CRMs), using both external calibration and standard addition method. The recovery degrees were in the range of 90–112% and 98–113% for external calibration and standard addition method, respectively, while the precision, expressed as relative standard deviation, was in the range of 4.8–14.5% and 4.6–13.3%. The results were similar to those obtained by microwave classical digestion, with recovery and precision in the range of 91–111%, and 6.7–13.7%, respectively.

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, contract nr. 15PED/2025, project number PN-IV-P7-7.1-PED-2024-0091, within PNCDI IV.

Hydrothermal carbonization of slurry after dark fermentation

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Key words: hydrothermal carbonization, hydrochar, liquid fraction, dark fermentation, slurry

Dark fermentation (DF) of kitchen waste (KW) produces hydrogen, volatile fatty acids and other by-products, leaving a slurry containing inoculum (digested sludge) and undecomposed KW. Hydrothermal carbonization (HTC) is the thermochemical process that accept moisture in the substrate. The main product of this process is hydrochar, but liquid and gaseous fractions are also produced. In this study the HTC of slurry after the DF process was carried out.

The HTC was performed in a reactor (4563M, Parr) with a working volume of 0.4 dm^3. The temperature of the process was 215°C and was maintained for 2.0 hours. The reactor was then rapidly cooled down. In the first step, the gas fraction was analyzed, followed by the liquid and solid fractions after separation by filtration. Three different substrates were used: slurry before DF, slurry after DF, and slurry after DF concentrated by centrifugation. The dry mass of the slurries (before DF, after DF, and concentrated after DF) were 3.2, 2.5 and 10.7%, respectively.

Based on the analysis, a higher hydrochar production yield was observed for the slurry after DF (40.5%) than for the slurry before DF (28.3%). Interestingly, the concentrated slurry after DF was characterized by the highest production yield of hydrochar (50.7%). Higher calorific values of the hydrochar was obtained, ranging from 16.1 to 18.2 MJ/kg. An inverse relationship was observed for the oil production yield. The highest production of the liquid fraction (70.4%) was obtained for the slurry before DF and the lowest one for the concentrated slurry after DF (48.3%). The pH of the liquid fractions ranged from 4.96 to 5.12. Total organic carbon (TOC) in the liquid fraction after HTC of the slurry before DF, after DF, and concentrated after DF was equal to 5.76, 6.52 and 9.19 g/L, respectively. The number of volatile organic compounds (VOCs) detected by the GC/MS system in the liquid fraction was in the ranged from 52 to 63. Such a complex mixture requires further treatment before it can be used in other processes. The main product in the gas fraction was CO_2, which means that the gas has little potential for use in other processes. The gas production yield ranged from 0.94 to 1.25%.

Acknowledgement
This research was funded by the National Science Centre (2021/43/B/ST8/00298).

Hydrothermal liquefaction of kitchen waste and digested sludge

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Key words: hydrothermal liquefaction, hydrochar, liquid fraction, kitchen waste, waste valorization

Hydrothermal liquefaction (HTL) is the thermochemical process which accept moisture in the substrate up to 99%. As a substrate we choose kitchen waste (KW) and digested sludge (DS) from the wastewater treatment plant. The aim of this study was to determine the yield and properties of products from HTL of KW and DS. The process was carried out in a pressure reactor (4563M, Parr) and control unit (4842, Parr). The temperature of the reactor during HTL was equal to 285°C, with a residence time of 3.5 hours. The working volume of the reactor was equal to 0.4 dm^3. Dry matter content of the KW and DS was 10.0% and 3.1%, respectively. After the process, the reactor was rapidly cooled down and the gas fraction was analysed. The solid fraction was separated from the liquid fraction by filtration. The quantity and composition of the solid and liquid fractions were also analysed.

Based on the results, we observed that the yield production of hydrochar from KW and DS was equal to 34.8 and 46.2%, respectively. The higher yield production of hydrochar from DS was due to the fact that DS contained 36.8% d.b. (dry basis) ash. In comparison, KW contains only 4.25% d.b. ash. The higher heating value (HHV) of KW was equal to 28.9 MJ/kg d.b., and was three times higher than that of DS. Yield production of the liquid fraction was 58.9 and 51.1% for KW and DS, respectively. The pH value after HTL was equal to 4.82 for KW and 8.34 for DS. The low pH was caused by the high content of acetic acid (4.55 g/L) in the liquid phase after HTL of KW. Total organic carbon (TOC) in the liquid fraction after HTL of KW and DS was 10.6 and 4.16 g/L, respectively. Analysis of volatile organic compounds (VOCs) in the liquid fraction using a GC/MS system detected 65 and 52 compounds after HTL of KW and DS, respectively. The gas production yield during HTL of KW and DS was 6.29 and 2.72%, respectively.

Acknowledgement

This research was funded by the National Science Centre (2021/43/B/ST8/00298).

Limit of detection for Se, Zn, Cu, Cd, Pb, Hg and As determination by white small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry and sample combustion compared to inductively coupled plasma optical emission spectrometry

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Key words: capacitively coupled microplasma, inductively coupled plasma, optical emission spectrometry, sample combustion

The limit of detection (LODs) is considered the most important figure of merit for a method, that determines the suitability and applicability for various samples using different analytical systems. The aim of the current study was the LODs evaluation of a green and white analytical method based on sample combustion (50 mg sample combustion in O_2 atmosphere followed by uptake in 0.1 mol L^{-1} HCl) and determination by small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry (SSETV-μCCP-OES). A number of 100 episodic emission spectra of elements for an integration time of 100 ms were recorded using the High-Speed Acquisition mode of the Maya2000 Pro microspectrometer Spectra Suite software. The analytical signal was obtained by 2D signal integration (time-wavelength) for different pixel numbers around the Central Pixel (CP) of the analytical line (CP, CP±1, CP±2 and CP±3). It was found that the best LODs (mg kg^{-1}) were obtained with CP±1 and CP±2, compared to CP strategy, namely 0.052 (Hg); 0.051 (Cu); 0.148 (Zn); 0.242 (Pb); 0.0042 (Cd); 0.322 (Se) and 0.173 (As). In terms of calibration curves linearity, it was found that the pixel numbers do not affect linearity, but affects the relative standard deviation of the blank (RSDB, %), becoming poorer as pixel numbers increases.

The LODs were also evaluated for inductively coupled plasma optical emission spectrometry (ICP-OES) with sample preparation based on classical microwave-assisted digestion in concentrated HNO_3 – H_2O_2 mixture. Arsenic, Hg and Se were determined by ICP-OES after hydride generation with $NaBH_4$ solution. In the case of both methods, the LODs were also discussed in the light of current European Legislations for maximum admitted concentrations of toxic metals in foodstuffs and food supplements. It was found that, generally the SSETV-μCCP-OES method is not suitable for toxic elements determination in vegetables and fruits, and it would necessitate its coupling with a preconcentration method, for example solid phase extraction (SPE) cartridges.

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, contract nr. 15PED/2025, project number PN-IV-P7-7.1-PED-2024-0091, within PNCDI IV.

Modelling Material Flow in Wastewater Treatment Using Automated Methods

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With increasingly stringent environmental regulations, accurate material balance calculations in wastewater treatment systems are essential for identifying necessary process improvements in industrial enterprises. This study presents an automated tool for determining the material balance of wastewater, incorporating key parameters such as chemical oxygen demand (COD), biochemical oxygen demand (BOD), fluorine (F), and adsorbable organic halides (AOX). Wastewater treatment typically involves multiple stages, each with distinct processes. For modelling these stages, it is necessary to know the quantities and qualities of input and output streams. The developed program evaluates both theoretical purification indicators and actual cleaning efficiencies after each stage of treatment. This dual approach bridges the gap between theory and practice, enabling direct comparison of predicted and observed performance, which was one of the purposes of this work at the beginning. The program's primary advantage lies in its ability to track quantitative and qualitative changes in wastewater parameters across treatment stages, to compare theoretical and real purification efficiencies, and to predict final effluent quality, supporting data-driven decisions in water resource management. With this tool water treatment specialists and environmental engineers can assess the performance of existing treatment facilities or optimizing operational processes in industrial settings. Also, its use helps to mitigating environmental risks through improved wastewater management. By enhancing the accuracy of purification forecasts, this model contributes to more sustainable wastewater treatment practices, aligning industrial operations with evolving environmental standards.

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

Multicriteria analysis of various CCS Technologies

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Carbon Capture and Storage Technology (CCS) is considered one of the most promising approaches for reducing CO_2 emissions produced by industry. There are numerous technologies available for CO_2 capture. Mostly used amine absorption, cryogenic separation or membranes that are still under development to be commercially available. Each of those technologies has its own advantages and disadvantages, particularly in terms of heat and electrical energy consumption. The aim of this study is to design CCS system for treating specific flue gas from industrial combustion process, to obtain CO_2 that meets required parameters for geological storage. Subsequently, a multicriteria analysis is applied to determine which technology is the most efficient from various perspectives, including economic, environmental, energy-related, and technological readiness level (TRL).

This study was supported by the Slovak Research and Development Agency under contract nos. APVV-18-0134 and APVV-19-0170. The authors acknowledge the financial support from the Slovak Society of Chemical Engineering and thank NAFTA a.s. for their valuable collaboration in conducting this study.

Ozonation-based processes for removal of Aminoglycoside antibiotic from wastewaters

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Keywords: Aminoglycosides, biodegradability, ozonation-based processes, UV treatment, wastewater

Global consumption of active medicinal substances represents an ever-increasing environmental problem due to the continuous introduction of low concentrations of active compounds into the environment and the indirect negative impact on non-target organisms. Established conventional wastewater treatment methods are ineffective in removing pharmaceutical micropollutants, so the use and implementation of advanced oxidation processes (AOPs) is crucial. Global human consumption of medicinal substances is estimated at between 100,000 and 300,000 tons with an average consumption of 15 grams per person per year. Due to incomplete metabolic processes, active substances can be excreted as parent compounds, main metabolites or a group of various metabolites. A certain proportion (30-90%) of antibiotics remains active after excretion, so the active substances can enter the environment indirectly and directly. The aim of the study was to use ozonation and ozonation in combination with hydrogen peroxide, Fe^{2+} and UV for pretreatment of wastewater, containing gentamycin sulphate. Gentamycin is persistent antibiotic with low metabolic rate in human applications. Model municipal wastewater was prepared by spiking gentamycin in different concentrations (50- 400 mg L^{-1}). Batch experiments were carried out at room temperature in a laboratory bubble column (300 mL). Ozone (4.5 g h^{-1}) was produced from oxygen p.a. in the Wedeco Ozone Modular HC8 ozone generator and fed into the reactor via a glass frit. The UV light source was a 6 W/42 V lamp (436.0 ± 9.6 lux). A set of three experiments was conducted and reduction of pH, COD, TOC, and BOD_5 were measured up to 120 min. It was confirmed that ozone and the combination of ozone/UV effectively remove chemical oxygen demand (COD) and total organic carbon (TOC) leading to increased biodegradation. The addition of hydrogen peroxide to ozonation did not improve the process, at most a similar removal efficiency was maintainedBy performing ozonation in combination with Fenton oxidation, the process was accelerated and the removal efficiency improved.

The impact of microplastics on the ozonation of wastewater containing the antibiotic amoxicillin

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Key words: amoxicillin, microplastics, ozonation, wastewater

This study investigated the ozonation of wastewater containing microplastics (MPs) made from several different materials, including polyvinylchloride (PVC), polypropylene (PP), polyethylene terephthalate (PET), polyethylene (PE), and rubber. Fraction size of utilized microplastics was less in the range of 0.8-1 mm. The initial phase involved ozonation of 500 mL of wastewater mixed with each type of microplastic (separately) at a concentration of 1 $g \cdot L^{-1}$. Chemical oxygen demand (COD) was measured at multiple intervals: 0, 5, 10, 20, 30, 60, 90, 120, 180, 240, 300, 360 minutes; to track the effectiveness of ozonation in degrading both the microplastics and organic pollutants in wastewater. Subsequently, the MP that demonstrated the highest ability to hinder COD removal was identified. Further investigations were conducted using this selected MP in a basic mixture ($pH > 10$), to evaluate how this variation influenced the ozonation process and overall degradation efficiency. COD was measured at the same intervals as in the initial experiments to compare the impact of pH adjustment on ozonation performance. In the final phase of the research, ozonation took place with a combination of the chosen MPs and amoxicillin, a common pharmaceutical contaminant. Similar to the prior steps, COD was measured at the set time intervals, and selected ions were determined at the beginning and end of ozonation to assess treatment efficiency. Additionally, total organic carbon (TOC) and inorganic carbon (IC) were also measured for each sample. COD removal followed comparable trends for WW with each MP and as expected, the treatment efficiency was highest in the raw WW, while the lowest was in WW with rubber. The efficiencies reached as high as 83 % for the ozonation of WW and generally after 6 hours it was in a range of 80‒70 % for all MPs samples. TOC removal also followed a common trend for ozonation of WW with each MP and reached the lowest value of 5.85 $mg \cdot L^{-1}$ for WW. Change in the pH was comparable for each ozonation, while only WW with PVC and rubber did not follow the trend. WW with PVC had a constant pH after the initial drop and with rubber it dropped to 6.50 after 90 minutes. Regarding values of IC, it was noted that the lowest values were measured in ozonated WW with rubber. It was concluded that MPs do have generally negative impact on ozonation process of WW.

Thermochemical conversion modelling of multilayer packaging waste using Aspen Plus®

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Key words: Multilayer packaging waste, Pyrolysis, Combustion, Global kinetics

Paper based multilayer packaging (PMP) is difficult to recycle due to its heterogeneous composition. Cellulosic fibers, with high recycling value, are recovered from the waste by hydro-pulping, whereas the remaining solid residues are mostly landfilled or incinerated. Pyrolysis is a thermochemical technique that can reduce this waste while producing valuable chemicals and energy. This study focuses on the reactor modelling of pyrolysis and combustion using Aspen Plus®. Global chemical kinetics were obtained from PMP's individual components and their mixture, adopting both model-free approaches (Friedman method and model-based compensation effect). Experimental data for kinetic modelling were collected utilizing a thermogravimetric analyzer for multiple heating rates (5, 10, 15, and 20 ^{o}C/min), under controlled nitrogen and air atmospheres. In the subsequent stage, the PMP's solid residue was thermally processed at bench scale to obtain the solid, liquid, and gas yields. Thereafter, robust pyrolysis and combustion models on Aspen Plus® for the PMP waste, using the process parameters acquired from the antecedent stages, were developed. Using the physicochemical properties, including the proximate & ultimate analyses, and heating values, the unconventional solids were defined to represent PMP mixture. A steady-state simulation of the waste thermochemical valorization was developed using Aspen Plus® V14. The process flow sheet comprised of four primary stages: hydro-pulping, drying, thermochemical decomposition and solid-gas separation. The detailed kinetic models and schemes were used to establish a robust feasibility analysis of PMP's pyrolysis against combustion.

Acknowledgements: The authors acknowledge the financial support by the French state managed by the National Research Agency in the name of France 2030 to conduct the French scientific program PAC-3R (ANR-22-PERE-0004). This work has also benefited from State aid managed by the Agence Nationale de la Recherche under the Programme d'Investissements d'Avenir with the reference ANR-18-EURE-0021.

Posters: Energy transition and circular economy

Anaerobic digestion as a solution for biowaste treatment in Slovakia

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Anaerobic digestion offers effective and green alternative to treat various types of organic waste. The process takes place in batch or continual reactors, in which organic substrates are transformed into biogas and digestate. There are two technological approaches that differs in total solids content in feedstock – wet (<15%), dry (>20%). Produced biogas is composed of ~55% methane, ~40% carbon dioxide, nitrogen, oxygen and hydrogen sulphide. Aim of this paper is to develop and compare mathematical models of continual and batch technology as well as evaluate the potential of building a new anaerobic digestion plant in multiple locations in Slovakia based on a feedstock analysis and usability of all products.

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

DECARBONIZATION STUDIES IN DISTILLATION COLUMNS

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Key words: decarbonization, distillation column, heat pump, C3 fraction

Distillation is considered one of the main separation and purification processes in industrial applications. It is widely used for separating different types of liquid mixtures. The energy efficiency of distillation columns is constantly advancing, to reduce the dependence on fossil fuels for heating these columns. Therefore, it is essential to address decarbonization in connection with distillation columns as well. In this work, we focused on the study of decarbonization of the distillation column used for the separation of a propane–propylene mixture, also known as a C3 splitter. Propane and propylene have similar boiling points and relatively high volatility, which results in high energy demands for their separation. C3 splitters usually operate at different pressure levels, with high-pressure columns (2 MPa) working in the conventional way, and low-pressure columns (1 MPa) usually operate with an integrated heat pump. The heat pump is used to recompress the overhead vapors, which provides heat through compression work and is subsequently used in the column reboiler. This study focused on several possible configurations of C3 splitters and their hydrocarbon footprint. It compares the decarbonization of different operational modes of the C3 splitter. In addition to comparing the amounts of emissions, an economic analysis was also performed based on the changes in energy prices, mainly for natural gas and electricity. This demonstrates, how the operating costs of different configurations of the C3 splitter would be affected by significantly fluctuating prices of enegies.

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

Fuels production from liquids after hydrothermal carbonization of kitchen waste – methane fermentation step

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Key words: kitchen waste, methane fermentation, hydrothermal carbonization

In recent years, due to the rapid increase in fuels costs, there has been a growing interest in the production of biofuels. One of the most common ways of the biofuel generation is the methane fermentation. However, there are still a lot of investigations conducted on the optimization of this process. One of the current trends is the production of hydrogen and methane from the substrate using two-step fermentation. Our earlier investigations showed that in two-step fermentation of kitchen waste produced more methane was than single-step fermentation – even though the gases produced in the first step were removed from the system [1].

In this study, kitchen waste (KW) was subjected to 0.5 h of hydrothermal carbonization at different temperatures – 180, 215 and 250°C. The liquids produced during this process were used as a substrate for the dark fermentation process. The remaining digestate was used as a substrate for the methane fermentation process, which was carried out in a static, periodic mode, under mesophilic conditions (37°C), using fermented sludge from the Wastewater Treatment Plant (WWTP) in Lodz as an inoculum. The volume of the biogas produced was measured by the displacement method, while the composition of biogas was measured by means of 8610C gas chromatography (SRI Instruments).

The obtained results showed that the hydrothermal carbonization temperature had a significant influence on the methane production from the generated liquids. The highest value of the Biochemical Methane Potential (BMP) was observed for the liquids generated in 180°C – 144±4 $mlCH_4/g_{TVSKW}$. It was 33% higher than for the liquids obtained in 25°C – 108±3 $mlCH_4/g_{TVSKW}$ but 47% lower than for the kitchen waste after the dark fermentation only (272±20 $mlCH_4/g_{TVSKW}$). Further increase of the temperature (to 215 and 250°C) resulted in a rapid decrease of the BMP value – to 44±3 $mlCH_4/g_{TVSKW}$ and 38±2 $mlCH_4/g_{TVSKW}$, respectively. As it can be seen, the use of hydrothermal carbonization as a hydrolysis step is not the most efficient method for increasing methane production. Moreover, the higher the hydrothermal carbonization temperature, the lower the BMP values.

Acknowledgement: Financial support from the National Science Centre (Poland) under project number 2021/43/B/ST8/00298 is acknowledged.

[1] Paździor K. et al., Kitchen waste valorisation–biofuels production, European Congress on Biotechnology 2024 – Book of abstracts, 160.

Hydrogen Strategy for RED III Compliance in a Refinery

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Key words: hydrogen, RFNBO, RED III, MCDA.

The European Union aims to achieve carbon neutrality by 2050. As part of the path toward a climate-neutral economy, environmental regulations are being continuously introduced and tightened. The latest Renewable Energy Directive (RED III), set to take effect from 2030, focuses on the energy, industry, and transport sectors. The Directive specifies the target share of renewable fuels in overall fuel consumption across these sectors. Notably, RED III requires a minimum 5.5% share of biofuels and 1% share of renewable fuels of non-biological origin (RFNBO), which can be generated through electrolysis using renewable energy. Hydrogen is an important component in refineries where it is utilized for polypropylene production and removal of undesirable elements such as sulfur or nitrogen from feedstocks. Currently, majority of hydrogen is produced by reforming processes. To comply with the RED III targets, a portion of hydrogen production should be substituted with RFNBO. In this work, several methods for achieving RED III targets are analyzed. RFNBO can be produced directly within the refinery. This can involve either generating a quantity of RFNBO sufficient to meet the refinery's own needs or facilitating production within the Slovak Republic. Alternatively, RFNBO can be sourced from countries where renewable energy is less expensive. Green ammonia may serve as an effective hydrogen carrier, which can be stored and subsequently decomposed in the refinery. Another scenario considers a situation in which RFNBO is neither produced nor purchased, which would incur penalties. To meet biofuel targets, biomethane can be acquired, contributing to lower carbon emissions. Additionally, hydrogen can be produced via thermal pyrolysis of natural gas or biomethane. During the pyrolysis reactions, CO_2 is not directly produced. Instead, solid carbon is formed, resulting in a lower carbon footprint compared to reforming process. Combinations of strategic pathways are evaluated and compared using a Multi-Criteria Decision Analysis (MCDA). The objective is to identify viable strategy for integrating renewable fuel solutions into refinery operations.

Acknowledgement

This work was supported by the Slovak Scientific Agency, grant no. VEGA 1/0151/24. Support by Slovak Society of Chemical Engineering is gratefully acknowledged.

Modeling and Experimental study of LOHC systems based on toluene mixtures

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Key words: Liquid Organic Hydrogen Carrier (LOHC), Hydrogenation, simulation study, parameter optimization

Hydrogen is one of the most promising energy carriers on the path toward a decarbonized future, due to its high energy density and clean combustion product. However, the efficient and safe storage of hydrogen remains a major technological challenge. Conventional storage methods are technologically complex, energy-intensive, and costly. A promising solution to overcome these disadvantages is the reversible binding of hydrogen to organic liquids, which enables chemically stable and safe storage (at atmospheric pressure and ambient temperature), while also allowing transportation via tankers, trucks, and pipelines.

In recent years, the applicability of various mono- and polycyclic aromatic compounds (e.g., toluene, n-ethylcarbazole, n-propylcarbazole, dibenzyl-toluene) and noble metal/oxide-supported and transition metal/oxide-supported catalysts has been investigated in LOHC systems. Among the carriers, toluene has been identified as the most suitable based on process parameters, and achievable conversions, while noble metal-based catalysts have proven to be the most favorable in terms of stability and selectivity.

The aim of the research work was to study and model the hydrogenation of toluene–methylcyclohexane mixtures, to analyze the effects of feedstock composition and process parameters, and to determine the optimal process conditions. A kinetic model was fitted to the experimental data, which served as the basis for constructing the reactor model for both hydrogenation and dehydrogenation. In both cases, the models showed a good fit to the experimental results.

This work has been implemented by the TKP2021-NKTA-21 project with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the 2021 Thematic Excellence Programme funding scheme. the work was also supported by the Aquamarine Plus Project, Complex Implementation of an Energy Project Proposal – Hydrogen-Based Developments at Hungarian Gas Storage Ltd., VHFO/80/2023-EM_CONTRACT.

Posters: Process design and process intensification

Optimization of lavender essential oil extraction: Method comparison and identification of key parameters

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Key words: *Lavandula Angustifolia*, essential oil, extraction, variable importance

Essential oils, as mixtures of different organic substances, play an important role in several industrial fields. Lavender essential oil is one of the most widely used worldwide. Its calming effect and pleasant fragrance make it a key ingredient in many cosmetic products. Essential oils are industrially extracted from plant raw materials by various physicochemical processes. During these processes, it is critical to assess the importance of extraction and plant cultivation conditions to optimize essential oil yield and composition of lavender oil.

The aim of our study is to compare how plant cultivation conditions, as well as extraction methods and parameters, influence the composition of *Lavandula angustifolia* essential oil. Different regression models were employed to estimate the essential oil composition and yield as functions of plant rearing conditions and extraction methods, and quantify the importance of each predictor variable.

In our work, lavender oil obtained through supercritical fluid extraction (SFE) and steam distillation was analyzed. The relative importance of extraction methods and parameters along with environmental factors (average temperature, precipitation) on the essential oil yield and composition were ranked with the parameters of the fitted regression models. The results indicate that environmental factors significantly influence the quality of the essential oil. When comparing the two methods, it can be concluded that supercritical extraction is more advantageous in terms of both composition and yield. However, its industrial use for producing essential oils is still not widespread.

Posters: Digitalization and process control

Modelling and Simulation of Reaction-Separation Processes using gPROMS ProcessBuilder

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Key words: Modelling, Simulation, gPROMS, Distillation, Reaction, Esterification, Pyrolysis

Modelling and simulation play a vital role in modern chemical engineering by enabling safer, more efficient, and sustainable process development. As industries face increasing pressure to optimize energy consumption, reduce emissions, and minimize waste, digital tools such as process simulators become indispensable. In this context, the concept of a *digital process twin* — a virtual replica of a real process — is gaining traction due to its potential for predictive analysis, optimization, and decision-making support. This work focuses on the application of the gPROMS ProcessBuilder to develop such digital twins.

Our methodology involves the creation of fundamental dynamic models of unit upstream and downstream operations based on physical knowledge of the process. The models are used to assess the effectiveness of the plant configuration and to observe system responses to step changes in operational parameters. Building on this foundation, we simulate more complex systems, such as coupled reaction-separation processes.

We study esterification of acetic acid in a continuous stirred tank reactor followed by a distillation column. Reaction kinetics follows the data from the literature. Different designs and operations of a distillation column were investigated to enhance the separation efficiency.

Secondly, we study the kinetics of plastic pyrolysis. Our work involves the estimation of model parameters. We employ the parameter estimation module within gPROMS ProcessBuilder, which enables kinetic models to be fitted to the experimental data through nonlinear regression. This enables the development of predictive models that can simulate the behavior of thermal decomposition processes under various conditions.

The simulations studied contribute to a deeper understanding of chemical systems and support future activities such as process optimization, control design, and the transition from laboratory to industrial applications.

Acknowledgments: This work is funded by the Slovak Research and Development Agency under the project APVV-21-0019, by the Scientific Grant Agency of the Slovak Republic under the grant 1/0263/25, and by the European Commission under the grant 101079342 (Fostering Opportunities Towards Slovak Excellence in Advanced Control for Smart Industries). RP acknowledges the financial support by the European Commission under the grant scheme NextGenerationEU project no. 09I03-03-V04-00530.

Multi-fidelity Modeling for Process Optimization in Refinery Operations

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Ensuring precise process monitoring in industrial refineries presents inherent challenges due to discrepancies between the continuous, high-frequency low-fidelity data streams from online sensors and the low-frequency high-fidelity laboratory measurements. In collaboration with Slovnaft, a.s., we construct a multi-fidelity soft sensor to address these inconsistencies, refining the accuracy of an online analyzer reading located on a downstream recycle of an alkylation unit. By leveraging multi-fidelity modeling techniques, we enhance real-time process control and improve decision-making in the operation room.

Both static and dynamic modeling formulations are integrated to evaluate their efficacy in process monitoring. Feature selection methodologies, encompassing Principal Component Regression, Partial Least Squares, LASSO, and Stepwise Regression, undergo assessment, with Stepwise Regression emerging as the most effective in balancing predictive accuracy and model interpretability. Our dynamic models explicitly incorporate time-lagged variables, capturing the intricate temporal dependencies introduced by recycle streams re-entering upstream processes. We employ a Gaussian Process, choosing multiple different covariance functions [1] to correct deviations between online analyzer data and laboratory measurements. A composite kernel effectively combines both stationary and non-stationary components, accounting for the different temporal behaviors and trends in the data.

The multi-fidelity models are able to capture the deviations between the low-fidelity and high-fidelity data. The dynamic multi-fidelity model is the best-performing, surpassing the static multi-fidelity model and the high-fidelity model. Compared to the currently deployed online analyzer, our multi-fidelity soft sensor achieves a noticeable, over 50 % enhancement in accuracy. These findings underscore the potential of multi-fidelity modeling in improving sensor reliability, minimizing dependence on laboratory sampling, reducing associated costs, and advancing decision-making strategies in industrial operations.

Key words: Data-driven modeling, Feature selection, Predictive accuracy, Data analysis

This work is funded by the Slovak Research and Development Agency under the project APVV-21-0019, by the Scientific Grant Agency of the Slovak Republic under the grant 1/0263/25, and by the European Commission under the grant 101079342 (Fostering Opportunities Towards Slovak Excellence in Advanced Control for Smart Industries). RP acknowledges the financial support by the European Commission under the grant scheme NextGenerationEU project no. 09I03-03-V04-00530.

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Posters: Separation processes and transport phenomena

Comparative Study of Membrane Processes for Lithium Carbonate Production: Electrodialysis vs. Donnan dialysis

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Key words: lithium carbonate, hollow fibers, Donnan dialysis, electrodialysis

In recent years, the demand for lithium has surged dramatically, primarily driven by the expansion of electromobility and the growing need for lithium batteries. Global projections indicate that by 2030, the demand for lithium batteries will be more than 11 times higher than in 2022. With limited access to primary lithium sources and lithium's designation as a critical metal in 2020, the recovery of lithium from secondary sources—such as spent batteries—has become increasingly important. Various technologies have been explored for this purpose, including ion exchange, electrodialysis, and Donnan dialysis, each presenting specific challenges that require optimization. Continued research and development are essential to enhance electrodialysis and other membrane processes while integrating multiple technologies to improve lithium recovery efficiency.

This study examines lithium carbonate recovery using two membrane-based technologies. The first approach employs electrodialysis metathesis with a module constructed from polypropylene ion-exchange membranes, followed by crystallization. The second approach utilizes Donnan dialysis with a module incorporating anion-exchange hollow fibers followed also by crystallization. The final crystal purities and key process parameters were analyzed and compared.

Both technologies demonstrate significant potential for lithium carbonate recovery, each offering distinct advantages. Electrodialysis excels in producing a high-purity intermediate product and can be adapted to various solution compositions. In contrast, Donnan dialysis operates at lower pressure and energy consumption, making it an energy-efficient alternative. However, both methods also have limitations—electrodialysis requires high energy input, while Donnan dialysis demands a higher purity of the feed solution. Further technological advancements are needed, and the optimal method depends on the quality of the input solution.

Acknowledgements

The work was carried out within the framework of the project "A long-term concept for the development of the research organization" supported by the Ministry of Industry and Trade of the Czech Republic, using the Membrane Innovation Centre infrastructure.

Design of reactive spray absorption column for decarbonization of flue gas

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Key words: CO_2 absorption, spray tower, reactive absorption, droplet modelling, carbon dioxide capture

Absorption is a separation method in which one or more gaseous components are selectively transferred into a liquid phase through gas–liquid contact. Key performance factors include interfacial area, mass transfer coefficients in both phases, and the concentration or pressure gradient of the absorbed components. In practice, several types of absorption columns exist, with the most common being packed bed columns, bubble columns, and spray towers.

This project focuses on developing a mathematical model for a one-dimensional NaOH spray tower absorber. In this setup, NaOH–water solution droplets fall under gravity through an upward-flowing, CO_2-rich gas stream. Each droplet is modelled as a small reactor, with its size, temperature, and composition tracked as it absorbs CO_2, evaporates water, and reacts to form Na_2CO_3.

The core of the model consists of a system of ordinary differential equations (ODEs) that describe droplet motion, mass transfer of CO_2 and water, heat balance (including reaction and evaporation), and the chemical reaction between CO_2 and NaOH. The gas-phase composition is also updated along the tower height to reflect CO_2 depletion and water vapor enrichment. This problem is formulated as a boundary value problem (BVP), with conditions specified at both the top and bottom of the tower.

The model equations were solved numerically. By varying parameters such as tower height, initial droplet size and number, and NaOH concentration in the feed, the model predicts CO_2 removal efficiency and the extent of NaOH conversion to carbonate.

The author Lukáš Halabuk acknowledge the financial support from the Slovak Society of Chemical Engineering.

Enzymatic synthesis of L-phenylserine in a semi-continuous milifluidic system

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Keywords: mili-reactor, enzymatic reaction, membrane reactors, L-phenylserine

Enzyme production is expensive, so we strive to make the best use of the enzyme during enzymatic reactions and preserve its lifetime. However, the enzyme is subject to rapid degradation, especially when organic solvents are involved in the enzymatic reaction. Preventing such degradation relies on modifying either the enzyme itself or the reaction conditions, ensuring the enzyme retains its activity for as long as possible. We investigated a potential adjustment of the experimental conditions in synthesizing L-phenylserine from glycine and benzaldehyde. Benzaldehyde and an aqueous glycine solution form a two-phase system. Enzyme degradation is believed to occur at the interface of these two phases. We used a dialysis membrane to dose the organic phase to prevent direct contact between the phases. Such an arrangement was tested in a semi-continuous reaction mode, realized in a milli-fluid chip, shown schematically in Figure 1. The body of the chip consists of two chambers separated by a dialysis membrane. One closed chamber contained the enzyme, and the other served as a flow-through chamber for the aqueous phase reaction mixture. The reactants diffused through the membrane into the closed chamber, where they enzymatically reacted, forming the product. The product (specifically, L-phenylserine) passed back through the membrane into the aqueous solution stream and was collected for analysis after exiting the chip. The advantage of this arrangement is not only preserving enzyme activity for a longer time but also its reusability, significantly decreasing the cost of the enzyme associated with phenylserine production.

Figure 1: Schematics of semi-continuous mili-fluidic chip with dialysis membrane

Modeling of Mass Transfer through an Ion-Exchange Membrane in Lithium Recovery by Donnan Dialysis

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Key words: lithium recovery, Donnan dialysis, ion-exchange membrane, ionic equilibria, mass transfer modeling

Lithium today has taken on growing importance with the rising global demand for its extraction, as it plays a significant role in the production of lithium-ion batteries for electric vehicles and renewable energy storage systems. Since primary resources are in finite supply, the need for efficient and sustainable methods of lithium recovery, particularly from waste streams, has grown in urgency. Apart from this, it is also important from an environmental perspective, as sustainable lithium recovery helps to restrict wastage, reduces the exploitation of natural resources, and helps in transition towards a more circular economy. One of the perspective techniques of lithium recovery is membrane crystallization using Donnan dialysis. In this process, a waste solution containing lithium cations and chloride anions is converted into lithium carbonate using anion-exchange membrane. Under the right conditions, lithium carbonate can be precipitated out from the solution. To optimize and better understand the process of lithium recovery, it is important to develop a mathematical model of Donnan dialysis ion transport mechanisms. This includes capturing the dynamic concentration changes within the both the ion-exchange membrane and the external bulk solutions. Mathematical modeling is an effective way of simulating the behavior of systems under varying operating conditions, reducing the need for extensive experimentation. In this context, the Nernst–Planck equation is the commonly used equation to describe the fluxes of charged species, with consideration of the combined effects of diffusion and migration in an electric field. When complemented by appropriate boundary conditions, electroneutrality constraints, and chemical equilibrium relations, the model provides a potent means for the analysis of ion selectivity, transport rates, and the formation potential of target compounds such as lithium carbonate. Additionally, such modeling facilitates process optimization and design and scale-up of efficient separation systems. During Donnan dialysis, the composition of the bulk solutions evolves over time as ions are selectively exchanged through the membrane. In open systems at atmospheric conditions, dissolved carbon dioxide equilibrates with the aqueous phase to form carbonate equilibria with species that include carbonic acid, and its dissociation products – bicarbonate and carbonate ions. These equilibria are sensitive to pH and ionic strength, and can affect both ion transport and the crystallization tendency of lithium carbonate. The model therefore includes dynamic changes in carbonate speciation in the bulk solutions in order to more accurately approximate real operating conditions.

Acknowledgments

This work was supported by the Slovak Scientific Agency, Grant No. VEGA 1/0658/24, and the Slovak Research and Development Agency under the contract No. APVV-22-0038 and VV-MVP-24-0365.

Purification of flue gas by new non-porous membranes

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Key words: flue gas purification, water condensing membrane, ionic liquid membrane

Abstract

One of the main sources of industrial emissions is combustion technology. In addition to solid waste, a number of compounds produced by combustion leave the system in the gaseous state. Currently, various methods are available for purifying flue gases released into the atmosphere to comply with emission standards fully. However, these technologies are now reaching the maximum limits for their separation capabilities.

This work aims to test various novel membranes using our unique apparatus for the separation of gaseous mixtures under the presence of humidity as in real systems. The presented automatized testing apparatus has a membrane cell with a variable area of tested membrane, water vapor saturators, and humidity sensors for all streams allowing fast modification of the experimental conditions and the whole system as well as gas analyzer allows measurement of acid gases as a CO_2 or SO_2 in the complex gas mixture.

In this contribution, we present the purification of feed gas to levels required by the legislation of the European Commission for thin film composite membrane with a polyamide functional layer in the presence of humidity. Other polymeric membranes based on ionic liquids and polymers with intrinsic microporosity were tested with single gases or their mixtures at various level of feed pressure and their performance (permeability, selectivity, stage-cut) will be presented.

Acknowledgement: This work was supported by grants of Czech Science Foundation No. 24-10288S.

Selectivity coefficients of ion exchange membranes and method of their determination

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Key words: ion selectivity; selectivity coefficient; ion exchange membrane; electrodialysis; desalination

To improve the performance of electrodialysis, it is crucial to investigate innovative approaches and techniques aimed at better characterizing membrane properties and predicting the desalination process. Selectivity serves as a useful tool for examining ion transport through ion exchange membranes, enabling the prediction of ion concentration reduction rates during desalination. Current research focuses on determining selectivity coefficients between monovalent and divalent inorganic ions using both homogeneous and heterogeneous membranes. The primary objectives were to validate the proposed method's applicability and assess the selectivity coefficients of different membranes.

A series of desalination batch experiments was conducted using a laboratory electrodialysis module with ten cell pairs. The feed solution consisted of a mixture of selected ions in various ratios. A constant voltage of 1V/cp was maintained across the membrane stack. To examine the validity range of the selectivity coefficients to be determined, different experimental conditions were tested, including temperature, voltage, ion concentrations, and the presence of organic non-dissociating compounds. Samples of the feed were collected during each batch and analysed to determine ion concentrations.

The evaluation indicated that the proposed method is applicable to both homogeneous and heterogeneous ion exchange membranes, and that the determined coefficients are valid across a broad spectrum of operating conditions. It was found that Ralex® heterogeneous membranes exhibit insignificant selectivity between mono- and divalent ions, whereas CEMs demonstrate even higher selectivity for divalent ions. The monovalent selectivity of Selemion ASVM membranes was confirmed; however, it was shown that fumasep® FAB-PK-130 membranes with hydroxyl-blocking properties possess significantly higher selectivity coefficients ($Cl^-/SO4^{2-}$).

Acknowledgements. The work was carried out within the framework of the project “A long-term concept for the development of the research organization” supported by the Ministry of Industry and Trade of the Czech Republic, using the Membrane Innovation Centre infrastructure.

Posters: Reaction engineering and catalysis

Preparation of nanofibrous catalysts for catalytic oxidation of volatile organic compounds by electrospinning

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Keywords: electrospun catalyst, polybenzimidazole, volatile organic compounds, catalytic oxidation.

One of the advanced methods for the preparation of heterogeneous catalysts is electrospinning, which offers unique possibilities in the production of catalytic supports. This technique enables the creation of materials with high surface area, controlled porosity, and tailored surface functionalities – all of which are key parameters for achieving high catalytic efficiency and selectivity. The nanofibrous structure of electrospun materials further enhances mass transfer and reaction kinetics, which is particularly critical for processes operating under high space velocities. Due to its versatility, electrospinning represents an effective tool for the preparation of innovative catalytic systems that can contribute to more efficient and sustainable environmental solutions in industrial applications.

Nanofibrous catalysts can be employed in the catalytic oxidation of volatile organic compounds (VOCs). This method is both effective and environmentally friendly, as it helps to reduce VOC emissions that contribute to air pollution. Suitable catalysts include materials impregnated with noble metals, such as platinum or palladium. Noble metal-based catalysts play a crucial role due to their high catalytic activity and stability.

This study presents a promising method for preparing efficient nanofibrous catalyst supports based on thermally and chemically resistant polybenzimidazole (PBI) via electrospinning. For model VOCs (ethanol, acetone, and toluene), the catalysts with low platinum content achieved high conversion rates (90%) at temperatures below 290 °C.

The results demonstrate the potential of these materials for applications in gas-phase reactions, such as VOC oxidation, with platinum nanoparticles serving as catalytically active sites. Unlike conventional pelletized catalysts, the high porosity of electrospun mats ensures easy accessibility of the platinum active sites to the reactants while maintaining a low-pressure drop in the catalytic bed.

Acknowledgement
The authors gratefully acknowledge the financial support provided by the Technology Agency of the Czech Republic (National Center of Competence, project no. TN02000044 “Biorefining and circular economy for sustainability”).

Posters: Material engineering and design

Development of Microrobots Using Stop-flow Lithography for Mechanostimulation of Encapsulated Cells

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Key words: cell encapsulation, stop-flow lithography, microactuators, mechanostimulation

The encapsulation of tissue cells within a three-dimensional (3D) hydrogel structure presents a valuable alternative to traditional two-dimensional (2D) cultivation methods, such as those utilized in Petri dishes or culture flasks. This 3D setup more accurately replicates the function of the extracellular matrix (ECM) and resembles the tissues found in live organisms. In tendon, ligament, and muscle tissues, the mechanical properties also play a crucial role, significantly influencing cell physiology. Both excessive and insufficient tension can lead to pathological cell behavior. The impact of mechanostimulation remains largely uncharted, and suitable hydrogels containing encapsulated cells can serve as a tool for establishing a controlled biomechanical environment, relevant for research into regenerative medicine and disease models.

This project aims to develop hydrogel microrobots capable of exerting force on encapsulated cells from the anterior cruciate ligament (ACL) to stimulate the production of cytokines—critical signaling and regulatory molecules. The encapsulation of ACL cells within hydrogels and the fabrication of microrobots for cell manipulation utilize the stop-flow lithography (SFL) technique, which involves a microfluidic chip, a photomask, and UV radiation. The microrobot is designed in the shape of a closed horseshoe, consisting of three components made from distinct materials: a rigid polyethylene glycol diacrylate (PEGDA) hydrogel, a thermoresponsive poly N-isopropylacrylamide (pNIPAM) hydrogel embedded with gold nanoparticles, and a septum composed of a biocompatible hydrogel containing encapsulated cells. Actuation is triggered by a 532 nm laser, which heats the gold nanoparticles through surface plasmon resonance, resulting in the contraction of the thermoresponsive hydrogel and the expansion of the septum housing the cells. In this study, four different methacrylated hydrogels were evaluated and compared: methacrylated hyaluronic acid (HAMA), methacrylated collagen (COLMA), methacrylated human platelet lysate (hPLMA), and hydroxyethyl methacrylate-modified dextran (DexHEMA).

Effect on surfactant solution stability of high saline brine water

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Key words: surfactant, polymer, brine water, enhanced oil recovery

The behaviour of surfactant and polymer solutions intended for tertiary oil recovery was investigated in the presence of various formation waters. The aim of the experimental work was to examine the dilution behaviour of solutions containing the surfactant SURF1 and the polymer POL1 in model formation waters with different salinities. These particular surfactant and polymer were selected based on their suitability for high-salinity environments.

Turbidity, transmittance, and stability tests were performed across a range of concentrations. The results indicate that divalent metal ions have a substantial impact on the solubility and stability of both surfactant and surfactant-polymer solutions. Significant changes in transmittance were observed during dilution at concentrations below 0.16 g/L, while precipitation occurred at higher concentrations. These findings provide valuable insights for optimising surfactant-based enhanced oil recovery (EOR) processes, particularly under conditions involving stratified waters with varying salinities.

Evaluation of biofouling rate of polypropylene water filters doped with composites of silver nanoparticles on halloysite

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Keywords: halloysite, silver nanoparticles synthesis, bacteriostatic additives, water filtration, melt-blow filter media

The filtration is a common process of water purification for industrial and domestic applications. Typical contaminations in water are particles (mineral, microplastics etc.), a variety of dissolved compounds (e.g. organics, ions, including heavy metals), and microorganisms. The ubiquitous bacteria, fungi and other species include their presence in the water, which creates potential hazards for human health and also affects downstream equipment, which includes equipment clogging, microbial corrosion, and coating of adsorbent or catalytic particles by forming a biofilm on their surface, etc. Non-woven filters manufactured using the melt-blown technique are widely used at various scales of filtration units. Over a long time of operation, the microorganisms captured inside the porous filter can intensively proliferate, which leads to reducing the operation time of the filter (determined by the maximum allowable pressure drop). This detrimental effect can be significantly reduced by incorporating of antibacterial compound into filtration materials.

The research aimed to evaluate the antibacterial effects of milled halloysite particles impregnated with nanoparticles (AgNP). The in-house prepared composites were dry-blended with polypropylene granules (1-2% by mass). The thermal resistance up to 300°C for additive was demonstrated, which confirmed its suitability for the melt-blown technique of filter manufacturing. The filtration experiments were carried out for 5-inch long filter cartridges using a controlled contamination of bacteria (Escherichia coli – Castellani & Chalmers ATCC 8739 strain) in a multipass operation mode. The concentration of living bacteria cells during filter testing corresponded to the concentration commonly observed in surface waters (i.e. was in the range 10^3-10^4 CFU/mL). The time needed to reach the pressure drop of 0.8 bar (the maximum achievable for the lobe pump used in the system) due to the biofouling of filter media was estimated. The time-dependent dP profiles were compared to unmodified polypropylene filters as a reference. The biofouling resistance for structures manufactured with halloysite-based composites has been proved: the reduction of the biofouling rate and the extension of time needed to reach the maximum allowable dP value were observed. Moreover, the elimination of the living bacteria from the water was confirmed for modified filter media using petri dish water cultivation and Microsnap test kit from Hygiena®.

The research was supported by the Polish National Centre for Research and Development, grant no. TECHMATSTRATEG-III/0005/2019-00

Influence of amino acid ionic liquids on morphology and sorption properties of HKUST-1

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Key words: Metal-organic frameworks, HKUST-1, amino acid ionic liquids, CO_2 adsorption

Metal-organic frameworks (MOFs) are a type of unique structures characterized by very large surface area, reaching even 6000 m^2/g. Thanks to that, MOFs could be useful in wide variety of applications like photocatalytic degradation of pollutants, hydrogen generation, drug delivery or as innovative and more effective in comparison to the commonly used materials – gas sorbents. The highly-porous MOF consisting of copper nodes and tritopic linker – 1,3,5-benzenetricarboxylic acid – known as HKUST-1, Cu-BTC or MOF-199, shows the carbon dioxide sorption capacity at remarkable level of 4.38 mmol/g. The influence of bio-based amino acid ionic liquid (AAIL), possessing high affinity towards CO_2, on MOFs morphology and sorption properties was investigated. Four AAILs (two 1-butyl-3-methylimidazolium- [BMIM] and two 1-ethyl-3-methylimidazolium-based [EMIM]) and one commercial ionic liquid used as reference (1-butyl-3-methylimidazolium bromide) were utilized to modify the chosen MOF. Two approaches of ionic liquid introduction were utilized, namely synthetical incorporation and post-synthetical impregnation. To validate the influence of AAILs on HKUST-1, techniques like Powder X-ray Diffraction and Fourier Transform Infrared Spectroscopy were used. Scanning Electron Microscopy was utilized to reveal the morphology of products. Size of the surface area was determined using Brauner-Emmett-Teller isotherm. Volumetric method was utilized to determine the adsorption capacity for CO_2. Sorption capacity at 25 °C for CO_2, CH_4 and N_2 was investigated within the pressure range of 0.5-10 bar with gravimetric unit. Incorporation of L-proline-based ionic liquid to the synthesis environment of HKUST-1 increased value of carbon dioxide sorption capacity reaching 6.26 mmol/g, giving 43% increase in comparison with pristine sample. Therefore, the selection of appropriate AAIL, as well as the method of introduction can lead to the improvement of sorption capacity and preservation of crystal structure of MOF.

Microstructured PDMS surfaces for bacterial adhesion control

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Replicating the intricate natural microenvironments is vital for developing advanced biomedical applications, yet conventional flat surfaces inadequately mimic these conditions, limiting progress in fields such as anti-biofouling and biomedical device design. To address this challenge, we engineered bioinspired microstructured surfaces on polydimethylsiloxane (PDMS) substrates, aiming to modulate bacterial adhesion behavior. Using maskless photolithography to create master molds and soft lithography for negative replication, we fabricated arrays of circular and rectangular microstructures in various sizes (down to 5 μm). Process parameters including exposure dose and baking times were optimized for structural precision. Topographical features were characterized using scanning electron microscopy and optical profilometry. The influence of surface topography on bacterial adhesion was then assessed using *Escherichia coli*, with adhesion levels quantified after incubation. Compared to flat PDMS controls, structured surfaces exhibited variations in bacterial adherence, depending on geometry and scale. Our findings underscore the potential of precisely engineered microstructured surfaces in controlling bacterial-surface interactions, opening avenues for applications in healthcare, bioengineering, and surface science.

Preparation of Ag colloidosomes from Pickering emulsions stabilized by mercaptocarboxylated Ag nanoparticles

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Key words: Ag, nanoparticle, Pickering emulsion, colloidosome

Colloidosomes are hollow superstructures with colloidal particle shells, and they can be prepared by using Pickering emulsion as templates. Specifically, crosslinking/thermal annealing of shell particles, evaporation of inner phases is reported as methods to prepare colloidosomes. Metal colloidosomes are recently developing fields which are potential for anticancer agent [1], photothermal materials [2], etc. Previously, colloidosomes with Fe_3O_4 shells were reported by Yang et al. [3]. It was also reported that Fe_3O_4 colloidosomes have better uptake into tumor cells and show higher stability in tumor cells than their building blocks [1]. However, the preparation of Fe_3O_4 nanoparticles mentioned in the above papers requires extremely high temperature; 300°C and occurs severe reaction during the nanoparticles formation. On the other hand, Ag and Au nanoparticles are also potential for anticancer agent, but Ag nanoparticles which sizes are nearly 10 nm has acute toxicity to mice [4]. In addition, raw materials of Au nanoparticles are very expensive. Therefore, we considered that using Ag nanoparticles (AgNPs) as building blocks can investigate milder and cost-efficient preparation of metal colloidosomes. The aim of this study is to prepare Ag colloidosomes from AgNPs-stabilized Pickering emulsion. First of all, we prepared AgNPs by phase transfer method. The prepared AgNPs were characterized by UV-vis spectroscopy and DLS, which showed its maximum absorption peak was at near 420 nm and their size distribution ranged from 1 to 100 nm, confirming that AgNPs were prepared. Second, we prepared Pickering emulsions using the AgNPs aqueous solution and chloroform as an organic solvent. Fluorescence microscopy measurement of the AgNPs-stabilized Pickering emulsions prepared by adding oil soluble Nile Red to their organic phase confirmed that O/W Pickering emulsion were prepared. Third, we prepared Ag colloidosomes by evaporation of inner phase of the Pickering emulsions by heating at 70°C. The prepared colloidosomes were characterized by DLS, optical microscopy, and SEM with EDS. As a result, ca. 1 µm hollow structures with Ag shells were observed. We observed similarities between the heated Pickering emulsions and creaming-occurred emulsions gained by just leaving them at room temperature for 3 days. Therefore, we successfully prepared colloidosomes with Ag shells by washing the creaming-occurred emulsions, without any heating processes. It was concluded that non-heating preparation of Ag colloidosomes were succeeded, which is milder and more cost-effective than conventional methods.

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Posters: Pharmaceutical engineering and processes

Biodegradable active substances release systems

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Key words: polyurethane, curcumin, biodegradation, drug delivery systems

Many of the modern drugs developed to combat various diseases cannot be easily used in postoperative treatment due to difficulties in achieving therapeutic concentrations of active agents in the injured areas. This problem is particularly acute in places with limited access, such as the urinary tract, brain, or paranasal sinuses. In order to meet the needs of both patients and doctors, a biodegradable polyurethane-based implant and hydrogel agar-based coating were developed to be placed in the right place during surgery. Combination of modeling, mechanical (bending, compression), structural (FTIR), thermal (DSC, MFR), surface (contact angle), microscopic (optical), degradation (2 M HCl, 5 M NaOH and 0.01 M PBS) analysis, release of the active substance and cell viability (MTT) allowed to assess the suitability of the developed material for the production of implants. Obtained polyurethanes were characterized with high mechanical strength ($\sigma > 20$ MPa), optimal biodegradability (>10 wt.% mass loss in 56 days), high release of hydrocortisone (up to solubility limit) and biocompatibility (>80% cell viability). The synthesized hydrogel coatings were also characterized with antimicrobial properties. However, before being used in clinical trials on humans, the developed materials must be first tested on animals to assess its impact on a living organisms.

Formulation and characterization of curcumin loaded oil marbles for improved delivery

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Keywords: Curcumin, Oil marbles, SMEDDS, Poor solubility

Curcumin, a bioactive compound derived from *Curcuma longa*, is one of many active pharmaceutical ingredients limited by poor water solubility. Despite its wide-ranging therapeutic properties, including anti-inflammatory, anticancer, and antioxidant effects, curcumin's clinical application is limited by its low bioavailability. To overcome these challenges, self-microemulsifying drug delivery systems (SMEDDS) offer a promising strategy by enhancing solubility and absorption through the formation of stable microemulsions in aqueous environments.

This study explores the development of a novel formulation of curcumin using Oil marbles, a type of semi-solid SMEDDS. The formulation consists of a mixture of oils, surfactants, and co-surfactants that, when exposed to water, spontaneously form microemulsions and facilitate the solubilization of curcumin, a lipophilic compound. Additionally, the Oil marbles are coated with a powder, combining the benefits of both liquid formulations, which enhance bioavailability, and solid dosage form, which improves handling and stability.

The focus of the research was to formulate curcumin into Oil marbles and assess its release behavior. The formulation process involved testing curcumin solubility in various oils, with ternary phase diagrams used to determine optimal oil, surfactant, and co-surfactant combinations that support efficient self-emulsification. The resulting microemulsions were characterized through droplet size analysis and visual inspection. Dissolution testing revealed significant improvements in the release kinetics of curcumin, highlighting the potential of this formulation to enhance curcumin's therapeutic effect.

Mini-tablets with Personalized Dissolution, Prepared by Fluid-Bed Granulation of Drug Nanosuspensions

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Key words: mini-tablets, fluid-bed, granulation, nanosuspension

Transforming poorly soluble active pharmaceutical ingredients (APIs) into nanoparticulate form is a well-established and effective strategy for enhancing their dissolution characteristics. Among the various methods available, wet-stirred media milling has emerged as a reliable and widely adopted technique for the preparation of API nanosuspensions. However, a significant challenge remains: converting these nanosuspensions into solid oral dosage forms without compromising their key properties, particularly their ability to re-disperse into fine particles upon administration.

In this study, a crude API was converted into a nanosuspension, which was then used in fluid-bed granulation to produce granules with adjustable dissolution properties. Polymeric binders, including hydroxypropyl methylcellulose (HPMC E5) and polyvinylpyrrolidone (PVP K30), were incorporated into the nanosuspension to aid granulation onto microcrystalline cellulose (MCC) or Pearlitol® CR-H substrates, which modulated the drug release rate.

The granules were subsequently compressed into minitablets, serving as modular building blocks for multi-unit dosage form (MUDF) capsules. By combining minitablets with varying dissolution profiles, it was possible to tailor drug release behavior, offering a simple yet powerful approach for personalized therapy.

This strategy not only provides flexibility in customizing dissolution kinetics but also supports the concept of precision medicine, where individualized therapy can be achieved by adjusting the combination of minitablets. The use of fluid-bed granulation with nanosuspension binders thus presents a scalable and adaptable platform for the manufacturing of personalized dosage forms.

Optimization of the permeation unit for advanced cell culture: Hostile territory for Caco-2 cells?

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Key words: Dissolution-permeation apparatus, Permeation unit, Cell culture

Oral drug delivery remains the most preferred and convenient route of administration yet predicting in vivo drug absorption continues to present significant challenges. While conventional in vitro dissolution tests effectively assess drug release from formulations, they fail to fully capture the complexity of the gastrointestinal environment—such as intestinal metabolism, drug transport mechanisms, and epithelial barrier function—that critically influence absorption. Incorporating cell-based models, such as Caco-2 cells, into the permeation unit enhances the physiological relevance of in vitro studies.

To better simulate the in vivo absorption process, we optimized a custom-built dissolution-permeation apparatus for cell-based experiments. The original permeation unit, not intended for cell culture, required several key modifications. These included the implementation of gas exchange via 3D-printed polycarbonate vents with PTFE filters to prevent contamination, revised sterilization procedures to avoid material deformation, and the replacement of cytotoxic components with biocompatible alternatives. A tissue culture-compatible polycarbonate membrane was introduced and coated with collagen to promote cell adhesion.

Two cultivation strategies were investigated: static and dynamic. In the static setup, initial failure to form a cell monolayer was attributed to toxicity from brass plugs and sealing grease, which were subsequently replaced with PVC-U plug and PTFE tape, enabling successful Caco-2 cell culture. The dynamic system holds promise but requires further optimization, particularly in identifying tubing materials durable enough to withstand long-term flow conditions.

Optimizing Freeze-Dried Drug Nanosuspensions: Role of Freezing Rate and Excipients

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Key words: Nanosuspension, Freeze-drying, Drug, Formulation

Poor aqueous solubility remains a major barrier in oral drug development, with approximately 80% of new drug candidates classified as BCS Class II or IV compounds [1]. These poorly soluble drugs often suffer from limited bioavailability, necessitating the development of advanced formulation strategies to improve their therapeutic performance. One such compound, indomethacin, a widely studied BCS Class II drug, was selected as a model in this study. To address its solubility and stability challenges, indomethacin was formulated as a nanosuspension and subsequently freeze-dried to produce a stable, easy-to-handle powder.

This study investigated the effects of formulation components, specifically surfactants and polymers, and freeze-drying process parameters on the redispersion of nanosuspensions. Stabilizer combinations were screened to identify optimal formulations, which were then freeze-dried under controlled conditions. Particular attention was given to the freezing step, where cooling rates were varied to optimize nanoparticle stabilization and minimize aggregation.

The lyophilized powders were characterized for particle size after redispersion, morphology, solid-state properties, and dissolution behavior. Results showed that both the choice of stabilizers and the freezing protocol significantly influenced the redispersion efficiency and dissolution performance. Cryoprotectants and faster freezing rates played pivotal roles in preserving nanoparticle integrity during the freeze-drying process.

Overall, this study demonstrates the importance of excipient selection and freezing conditions in maintaining nanosuspension quality after freeze-drying. Optimizing these parameters offers a promising approach to enhance the stability and bioavailability of poorly soluble drugs.

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Spray-drying of inhalable prodrug-enzyme systems with antibacterial properties

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Key words: spray drying, inhalation, antimicrobial, allicin, prodrug

Rising numbers of multidrug-resistant bacteria and the desire to avoid systemic drug exposure are among the key challenges of current pharmaceutical development. Inhalable powders with prodrug-enzyme systems may contribute to progress in both areas, using natural defence mechanisms as inspiration. For instance, plants of the genus *Allium*, i.e., garlic, onion, leek, rely on the broad and strong antimicrobial effect of thiosulfinates. They are synthesized from sulfoxides, i.e., prodrugs, using the enzyme alliinase. This happens only when the plant cells are attacked by microbes. Moreover, thiosulfinates are volatile and unstable, leading to hindered onset of microbial resistance. However, unstable compounds cannot be put safely into a drug product with long-term stability. Therefore, we propose to formulate sulfoxides and alliinase into inhalable spray-dried powders, where the reaction is triggered by contact with the moist environment of the lungs. Delivering antibiotics directly to the place of action and avoiding systemic drug exposure is of high importance here because it decreases the necessary dose and limits the damage caused to the gut microbiome. Moreover, thiosulfinates are the only antibiotics active in a vapour state[1], which may enable them to overcome mechanical barriers posed by chronic lung diseases.

In this work, we used the three-fluid atomization nozzle to spray dry powders containing alliinase and sulfoxide alliin in all particles, together with carrier maltodextrin. This nozzle allows for the entry of two separate feeds, i.e., alliin-maltodextrin and alliinase-maltodextrin, which only meet at the nozzle orifice. This approach limits the alliin-alliinase contact in liquid state, while enabling their presence in one particle and, thus, facilitating thiosulfinates production at the place of action. We evaluated the effect of different designs on the amount of thiosulfinates produced during spray drying. Moreover, we studied the antibacterial effect of prepared powders and their storage stability. In the future, we plan to test the deposition and antibacterial effect of these powders in a simplified lung model.

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This work was financially supported by the Czech Science Foundation (GAČR), project No. 23-07356S.

There is “something” in the air: an overview of allicin-based antibacterial materials

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Key words: allicin, antibiotics, encapsulation, enzyme, spray drying, 3D bioprinting

The rising prevalence of multidrug-resistant (MDR) bacterial strains constitutes a significant threat to modern global society. Unfortunately, the practical and financial challenges associated with developing new antibiotics have already led many pharmaceutical companies to shift their focus toward different, more cost-effective and profitable products. On the other hand, garlic (*Allium sativum*) has been used in various forms and cherished worldwide as a universal natural remedy. Allicin, produced in garlic enzymatically from its stable precursor (alliin) due to mechanical damage, has gained significant scientific attention for its exceptionally broad range of therapeutic effects. A combination of the short half-life, high reactivity and non-specificity to particular proteins is a reason most pathogens cannot cope with allicin's mode of action and develop effective defence mechanisms. Furthermore, it has been demonstrated that allicin can induce transient pore formation in biological membranes, which renders pathogens more vulnerable. The synergistic use of antibiotics and allicin proved to be more effective than monotherapy, enhancing antibacterial action, lowering biofilm levels, and reducing dosage and associated negative toxic effects. Thus, using a combination of allicin with common antibiotics may serve as a viable solution to address drug resistance in infectious diseases.

Drawing inspiration from the antibacterial properties of allicin and its efficacy against multidrug-resistant (MDR) bacterial strains in both liquid and gas phases, we implemented a variety of strategies to replicate the natural concept of substrate-enzyme compartmentalisation. We developed materials for the on-demand synthesis of allicin in several forms, including flexible casted films, 3D bioprinted structures of various geometries, core-shell beads with diameters in the hundreds of microns achieved through encapsulation, and spray-dried microparticles with diverse internal structures, suitable for topical application or deep lung inhalation. We assessed the cytotoxicity of these materials against relevant cell cultures that reflect the intended application site and confirmed their antibacterial effectiveness using both standard and non-contact testing methods explicitly developed for this purpose in our laboratory. We aim to show that different techniques can be used to encapsulate both enzyme and substrate in various forms, enabling the synthesis of antibacterial allicin for a specific application.

Yeast *β*-glucan particles and composition of their core

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Key words: *β*-glucan, *β*-glucan particles, drug delivery, Bradford assay

Yeast-derived *β*-glucan particles (GPs) make a promising material for use as a bioactive drug carrier for targeted drug delivery. It has been discovered before that GPs are phagocytosed by immune system cells in the intestine, macrophages specifically, which opens new opportunities of targeted drug delivery. Data from the literature and our laboratory suggest that such particles contain a residue in their centre, which is never discussed in the literature. Such a residue could represent an obstacle for pharmaceutical use of GPs and was, therefore, examined. The composition of the residue remained unknown until the use of Confocal Raman Microscopy, which revealed that it is made of glycogen and protein. Both of these were quantified and attempts to get rid of them were carried out. Quantification of protein content was carried out using Bradford assay and quantification of glycogen was carried out using *α*-amyloglucosidase enzyme and followed by assaying the liberated glucose using an oxidase/peroxidase/*o*-dianisidine kit. Glycogen and protein removal was attempted enzymatically and in case of glycogen by rehydration of yeast in nutrient-poor medium prior to GP preparation. Attempts at removal of glycogen were mostly successful, attempts at protein removal proved to be more difficult and were successful only partially.

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