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2026

PROCEEDINGS

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#SSCHE2026

SLOVAK SOCIETY OF CHEMICAL ENGINEERING

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

PROCEEDINGS

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Contents

Program

Plenary lectures

Lectures

Lectures: Energy transition and circular economy

Lectures: Bioprocess and biotechnology

Lectures: Risk management and process safety

Lectures: Environmental chemical engineering

Lectures: Process design and process intensification

Lectures: Digitalization and process control

Lectures: Separation processes and transport phenomena

Lectures: Reaction engineering and catalysis

Lectures: Material engineering and design

Lectures: Pharmaceutical engineering and processes

Lectures: Energetická transformácia priemyslu & Zhodnocovanie vedľajších prúdov z výroby (SK industry session)

Posters

Posters: Environmental chemical engineering

Posters: Reaction engineering and catalysis

Posters: Material engineering and design

Posters: Pharmaceutical engineering and processes

Program

Tuesday

13:00–20:00	**Arrival of participants; Registration**

17:00–18:00	**Hall A: Conference opening; Plenary lecture I (Chair: Mário Mihaľ, Ján Janošovský)**

17:00	**Conference opening**
17:15	From waste to value - Sustainable recycling of ashes and flu gas CO2 by mineralization in an advanced pH shift process (*Voigt, A.*)
18:00–20:00	**Dinner**

20:00–23:00	**Poster session; Welcome drink**

1	A comparative study of various Pr(La)SrBaCeCo(Ni)Ox compounds for total oxidation of ethanol (*Balabánová, J., Jirátová, K., Koštejn, M.*)
2	A comparison of the sorption properties of starch from Horse Chestnut (Aesculus hippocastanum) and London Plane tree (Platanus acerifolia) fruits. (*Ocieczek, A.*)
3	Advanced SiO2-based adsorbent for CO2 capture (*Setnickova, K., Šabata, S.*)
4	Analysis of the Efficiency of Acid Thermohydrolysis of Lignocellulosic Biomass (Willow Chips) Using Conventional and Microwave Heating in the Biogas Production Process (*Nowicka, A., Dudek, M.*)
5	A Practical Approach to Anomaly Detection in Industrial Data (*Arbetová, P., Fáber, R., Ľubušký, K., Paulen, R.*)

62	The significance of hydrogen concentration monitoring in primary coolant circuits (*Moucha, T., Bouřa, A., Macas, J.*)
63	Toward Green NH3 Electrosynthesis: Nanocatalysts, 3D-Printed Electrodes, and Electrolyzer Design (*Givirovskiy, G., Givirovskaia, D., Nadeem, U., Piili, H., Repo, E.*)
64	Waste biomass-to-electrode materials: biochar-based carbon for electrochemical flow systems (*Beliančínová, K., Frišták, V.*)
23:00	**End of poster session**

Wednesday

08:40–12:20	**Hall A, Lectures: Separation processes and transport phenomena (Chair: Dr. Mário Mihaľ, Dr. Pavel Izák)**
08:40	Determination of sorption selectivity in ion exchange membranes and its influence on ion transport (*Hlavatý, L., Sedláková, E., Sedlák, L., Červeňanský, I., Markoš, J.*)
09:00	Effect of non-ionic surfactants on velocity of single rising bubble (*Shirokov, V., Orvalho, S., Kosior, D., Zawała, J., Basařová, P.*)
09:20	Electrodialytic separation of bio-based volatile fatty acids (C2-C6) (*Rózsenberszki, T., Koók, L., Bakonyi, P.*)
09:40	Free-Flow Electrophoresis: An experimental platform for continuous separation of enantiomers (*Sklenář, A., Sauer, L., Přibyl, M.*)
10:00	Gas Sorption in PEEK-Ionene Composite Membranes for Flue Gas Purification (*Izák, P., Stanovský, P., Friess, K.*)
10:20–10:40	**Coffee break**
10:40	Investigation of the vapor-liquid phase equilibrium of a binary mixture of eucalyptol and various alcohols (*Vészi, A.*)
11:00	Separation of succinic acid from the mixture of organic acids using pertraction (*Mihaľ, M., Stoláriková, Z., Červeňanský, I., Markoš, J.*)
11:20	Microfluidic systems for separation and preconcentration of ion species using the ion depleted zone (*Škrhák, M., Slouka, Z.*)
11:40	Phytosterol isolation from vegetable oils: Methods and Valorization Potential (*Fromel, R., Janošovský, J., Mareček, L.*)
12:00	Study of Donnan Dialysis for the Recovery of Valuable Substances from Wastewater (*Tomášik, M., Hlavatý, L., Červeňanský, I., Markoš, J.*)

12:20	**End of session**

08:40–12:20	**Hall B, Lectures: Bioprocess and biotechnology (Chair: Prof. GONCAGÜL SERDAROĞLU, Dr. László Koók)**
08:40	Cellulose-based ionogels as novel membrane materials for microbial fuel cell applications (*Koók, L., Szabolcs, S.*)
09:00	Chromatographic Purification of Polyphenolic Compounds from a By-Product of Rapeseed Protein Isolation (*Mazanová, M., Koššuthová, A., Antošová, M., Polakovič, M.*)
09:20	Enhancing Caprolactone Production via Multienzyme Cascade in E. coli (*Holienka, K., Illeová, V., Polakovič, M.*)
09:40	Evaluating microbial desalination kinetics and efficiency at various substrate loadings and initial salinity (*Nagy, K., Koók, L.*)
10:00	Hydrogel Microactuators for Laser-Induced Mechanical Stimulation in 3D Cell Culture (*Zlatník, J., Mamedova, A., Heidenberger, J., Rothbauer, M., Tokárová, V., Řehoř, I.*)
10:20–10:40	**Coffee break**
10:40	Preparative chromatographic separation of polyphenols from black chokeberry and sea buckthorn with macroporous resins (*Koššuthová, A., Mazanová, M., Macias - Garbett, R., Antošová, M., Jágr, M., Polakovič, M.*)
11:00	The substitution group and solvent effect on the chemical behavior of chlorine-functionalized Ferulic acid (*SERDAROĞLU, G., KARAKUŞ, N.*)
11:20	Spray-dried bioactive microparticles for antimicrobial applications (*Nováková, N., Fiřtová, Š., Dvořák, V., Maršík, D., Mašková, L., Maťátková, O., Kašpar, O., Tokárová, V.*)
11:40	Small-scale bioreactors: challenges in experimental determination of hydrodynamic stress in stirred vessels (*Behner, A., Bursík, V., Trunov, D., Šoóš, M.*)
12:00	The 2-phenylacetic acid derivatives functionalized with NH2 and -NO2 groups: FMO, NBO, UV-Vis, Pharmacokinetics studies (*SERDAROĞLU, G.*)
12:20	**End of session**

12:00–14:00 **Lunch**

14:00–15:20 **Hall A, Lectures: Environmental chemical engineering (Chair: Prof. Tapio Salmi, Dr. Christof Lanzerstorfer)**

14:00 Application of Natural Deep Eutectic Solvents for the Extraction of Bioactive Compounds from Rapeseed Meal (*Amjad, S., Rabiej-Kozioł, D., Szydłowska-Czerniak, A.*)

14:20 Combined Physicochemical Processes for Quaternary Wastewater Treatment (*Jurík, J., Bodík, I.*)

14:40 Energy assessment of brine processing (*Hríbik, D., Variny, M., Červeňanský, I.*)

15:00 Zinc Speciation in Dust from a Secondary Dedusting System of the Basic Oxygen Furnace (*Lanzerstorfer, C.*)

15:20 **End of session**

15:20–15:40 **Coffee break**

15:40–17:00 **Hall A, Lectures: Material engineering and design (Chair: Prof. Tapio Salmi, Dr. Christof Lanzerstorfer)**

15:40 Crystal Engineering of Low-Dimensional Metal Halide Hybrids for In-Memory Computing Technologies (*Abdi, G., Alizadeh, A., Mazur, T., Cechosz, E., Sławek, A., CAUS, D., Szaciłowski, K.*)

16:00 Electronic Structure and Reactivity Descriptors of BN-Doped Naphthalimide-Carbazole Bipolar OLED Emitters: A DFT/TD-DFT Study (*KARAKUŞ, N., SERDAROĞLU, G.*)

16:20 Integration of microstructured surfaces into microfluidics for dynamic biofilm research (*Nguyen, V., Kříž, F., Nováková, N., Kašpar, O., Tokárová, V.*)

16:40 Processing-Driven Porosity Engineering in Resorcinol Formaldehyde-Derived Carbon Gels for High-Performance Supercapacitors (*Chavhan, M.*)

17:00 **End of session**

13:30–16:30	**Hall B, Priemyselná sekcia (SK industry section)**

13:30	**Otvorenie priemyselnej sekcie**
13:40	Dekarbonizácia priemyslu: 6,4 MW strojovňa tepelných čerpadiel na odpadové teplo (*Michalec, M.*)
14:00	Transformácia zemného plynu na zelenú energiu: Komplexné riešenie pre teplo, chlad aelektrinu (*ILLITH, R.*)
14:20	Získávání energií zodpadních vod technologií HUBER ThermWin (*Musil, J.*)
14:40	Komplexná valorizácia vedľajších prúdov a odpadov: Od nápadu k realizácii (*Janošovský, J.*)
15:00	Zlievarenský piesok v cirkulárnej ekonomike: limity, príležitosti a reálna implementácia (*Cedzo, L.*)
15:20–15:45	**Coffee break**
15:45–16:30	**Panelová diskusia**
16:30	**Koniec priemyselnej sekcie**

17:05–18:05	**Hall A, Plenary lecture II, Poster award announcement (Chair: Dr. Mário Mihaľ)**

17:05	Novel frontiers in circular and sustainable brine mining (*Cipollina, A.*)
17:50	**Poster award announcement**

19:00–03:00	**Conference party**

Thursday

08:40–10:40	**Hall A, Lectures: Energy transition and circular economy (Chair: Prof. Janusz Lasek, Dr. Petr Mazúr)**
08:40	Carbon Capture, Utilization and Storage (CCUS) perspectives in Indonesia and Visegrád Countries (*Raynaldi, M., Harangozo, G., Variny, M.*)
09:00	Aqueous organic redox flow batteries for high-temperature operation (*Mazúr, P., Spurný, M., Števuliak, M., Kubáč, L., Černý, J.*)
09:20	Retrofitting and Optimization Strategies for Decarbonizing District Heating Systems (*Turinič, N., Variny, M.*)
09:40	Analysis of hybrid energy storage systems using post-mining infrastructure, including day-ahead market (DAM) and system operating cycle characteristics (*Głód, K., Supernok, K., Czardybon, A., Lasek, J.*)
10:00	Quantifying the digitalisation contribution to the management of increasing RES absorption in the electricity market: the case of Slovakia (*Szaryszová, P., Kuhnová, L., Variny, M.*)
10:20	Comparative Performance of Lithium-Ion, Sodium-Ion, and Lead-Acid Batteries in a Solar Photovoltaic System Using MATLAB/Simulink (*Bastos, I., Quinelato , L., Kienberger, T.*)
10:40	**End of session**
10:40–11:00	**Coffee break**

11:00–12:20	**Hall A, Lectures: Reaction engineering and catalysis (Chair: Prof. Janusz Lasek, Dr. Petr Mazúr)**
11:00	Co-solvent free conversion of biomass-originated levulinic acid to -valerolactone: from molecular level to process design (*Mika, L., Árvai, C.*)
11:20	Continuous Xylitol Production on Solid Foam Catalyst: Mass Transport and Kinetic Modelling (*Araujo Barahona, G., Ciaramella, M., Eränen, K., García Serna, J., Russo, V., Murzin, D., Salmi, T.*)
11:40	Biomass to useful molecules From batch to continuous operation with the aid of structured catalysts and reactors (*Salmi, T., Araujo Barahona, G., Mastroianni, L.*)

12:00	Phosphine-free Heck coupling reaction, in 1,4-pentanediol as an alternative biomass-derived medium (*Árvai, C., Mika, L.*)
12:20	**End of session**
12:00–14:00	**Lunch**

14:00–15:40	**Hall A, Lectures: Risk management and process safety & Process design and process intensification (Chair: Prof. Michal Přibyl, Dr. Edit Cséfalvay)**
14:00	Dynamic Modelling Approach to Identifying Critical Operating Conditions in Ammonia Synthesis (*Valiyeva, K., Jelemenský, L., Myšiak, J.*)
14:20	Influence of collision velocity on triboelectric charging of polyolefin particles (*Perner, J., Jantač, S., Sklenářová, J., Drápela, M., Pelcová, J., Zubov, A.*)
14:40	Alignment of characteristic times in microfluidic systems for the preparation of enantiomers (*Sauer, L., Sklenář, A., Vobecká, L., Slouka, Z., Kralik, D., Přibyl, M.*)
15:00	Make-up water production from laboratory-scale experiments and industrial-scale design (*Al-Madanat, Q., Cséfalvay, E.*)
15:20	Application of GPU-Based Computation in Chemical and Safety Engineering (*Halabuk, L., Labovský, J.*)
15:40	**End of session**
15:40–16:00	**Coffee break**

16:00–17:00	**Hall A, Lectures: Pharmaceutical engineering and processes & Digitalization and process control ((Chair: Prof. Michal Přibyl, Dr. Edit Cséfalvay)**
16:00	Characterization and identification of anthocyanins in natural extracts (*Karaba, S., Pätoprstý, V., Kopáčová, M., Filčáková, A., Tomash, J., Rajniak, P.*)
16:20	Study of the Stochastic Nature of Nucleation in Freeze-Drying (*Filčáková, A., Shepherd, J., Annus, J., Karaba, S., Rajniak, P.*)

16:40	Multi-Emissivity Measurement Device for Monitoring and Control of Radiative Heating Systems (*Pipíška, A., Rejl, F.*)
17:00	**End of session**

17:05–18:00	**Hall A, Plenary lecture III, Conference closing (Chair: Dr. Mário Mihaľ)**
17:05	Chemical engineering of ion-exchange membranes: from biosensing to electrodialysis (*Slouka, Z.*)
17:50	**Conference closing**
18:00–20:00	**Dinner**

Friday

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

Plenary lectures

Chemical engineering of ion-exchange membranes: from biosensing to electrodialysis

Zdeněk Slouka[1]

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Keywords: ion-exchange membranes, reaction-transport phenomena, biosensing, preconcentration, ion separation, electromembrane processes

Abstract

Ion-exchange membranes are selective materials traditionally employed in electromebrane processes, such as electrodialysis, for the removal of small ions from processed water solutions. However, when viewed as materials that allow one to control the flux of ionic species by externally applying a DC electric field, the range of potential applications significantly widens. The reason for this is the interesting but rather obscure behavior of ion-exchange membranes in the electric field. Especially at the interface between the given membrane and the processed solution, the observed behavior is determined by the complex interplay of various reaction-transport phenomena, such as diffusion, migration, electroconvection, gravitational convection, pressure-driven convection, and acid-base reactions facilitated by a strong local electric field. Depending on the properties of the given membrane and the ionic species in the water solution, those processes can attenuate or amplify, providing a largely unexplored space for chemical engineers.

To unveil and describe these complex systems, we combine experimental and theoretical approaches to understand the spatiotemporal evolution of ion-exchange systems under various conditions. Specifically, we use microfluidic technologies to construct experimental systems that not only allow us to measure integral characteristics, such as polarization curves and the achieved degree of desalination, but also to reconstruct time- and spatially resolved maps of important quantities, such as velocity, concentration, or electric potential. The experimental observations are then explained in the context of numerical simulations of formulated mathematical models, based on conservation of momentum, species, and energy, and the Poisson equation of electrostatics, providing an inspiration for potential applications of ion-exchange membranes. These applications indeed include biosensing, biomolecule preconcentration, molecular separation, ionic separation, and preconcentration or chemical production.

In the talk, we will focus on combining fundamental engineering research on ion-exchange membranes with their potential applications.

From waste to value - Sustainable recycling of ashes and flu gas CO2 by mineralization in an advanced pH shift process

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Limited resources and climate change, these two major challenges are currently driving the chemical industry towards change and innovation. There is a clear need to find alternatives to fossil fuel to still produce all necessary goods for our society. One effective source of carbon should be carbon dioxide which accumulates in our atmosphere driving temperatures up everywhere on the planet. But at 420ppm the concentration of CO_2 is very low and large and expensive efforts are needed to capture the CO_2 directly from the air. Much higher CO_2 concentrations are available in processes where carbon oxidation is applied, namely in a typical power plant for heat and electricity production. The flu gas contains up to 15% CO_2 and in the coal-fired power plants, another source for an alternative process idea is available as well, the ash from the carbon burning process. At the moment, flu gas and ash are considered as waste, to be disposed of, with an economically and environmentally negative impact. But this can be changed and I will present an innovative process idea of extraction, filtration, precipitation and separation using the "wastes" as educts and a clever pH-shift process to produce a valuable product applicable for example in the paper and color industry.

The main steps are the extraction of Calcium ions from the ash under mild acidic conditions at around pH 2-4, the filtration of the slurry to obtain a clear Calcium ion containing solution, the shift of pH to mild basic conditions of pH 9-11, the addition of CO_2 to induce a reaction between the Calcium ion, Ca^{2-}, and the carbonate ion, $(CO_3)^{2-}$, the precipitation of $CaCO_3$ as a solid and finally the separation of the solid particles as the product. As straightforward as this sounds, a number of small and big obstacles along the way will be shown and also some detours highlighted.

The presented research is part of a collaborative effort in a German priority program SPP2364 and additional information can be found in a recent publication [1].

[1] Volker Bächle, Chinmay Laxminarayan Hegde, Andreas Voigt, Kai Sundmacher and Marco Gleiß: *Tailings as a Source for Generating Valuable Magnesium and Calcium Carbonates by Leaching and Carbonization*, Industrial & Engineering Chemistry Research **64**(24) 12064–12073 (2025). https://doi.org/10.1021/acs.iecr.5c00797

Novel frontiers in circular and sustainable brine mining

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Abstract

Global desalination capacity generates approximately 90 million m^3/day of industrial waste brine: a potential source or minerals and raw materials, currently totally unexploited. While, conventional minerals extraction is hindered by high environmental costs and geopolitical dependencies, particularly for Magnesium (classified by EU as a Critical Raw Material), novel frontiers in sustainable brine mining advocate for a shift toward the circular processing of brine and bitterns (concentrated brines remaining after natural salt crystallization) to secure access to these materials while adhering to the highest environmental standards. In this framework, the University of Palermo (UNIPA) has played a central role in developing cutting-edge technologies, validated at the pilot scale, to recover CRMs and other valuable resources from brine, within international EU projects as SEArcularMINE, Water Mining and MareMag LIFE.

The technological core of this approach involves magnesium recovery through Multiple Feed Plug Flow Reactors (MF-PFR), within circular schemes ensuring full sustainability by in-situ chemicals generation via Electrodialysis with Bipolar Membranes (EDBM), which produces sodium hydroxide (NaOH) and hydrochloric acid (HCl) solutions directly from brine, achieving a circularity potential of over 99%. These systems enable the production of magnesium hydroxide ($Mg(OH)_2$) with high purity (>99%) and exceptional process yields (>99.9%), yet keeping the specific electrical consumption to very low values (2-3 kWh/kg of $Mg(OH)_2$ produced), providing a sustainable alternative to traditional mining.

The gained experience from lab-scale research to pilot plants operating in real operational sites in Lampedusa and Trapani will be presented, demonstrating the technical feasibility in operational environments and technology readiness levels advancements from TRL 4 to TRL 7.

Finally, Life Cycle Assessments (LCA) indicate how these circular approaches can reduce the emission of relevant amounts of CO_2 and save significant freshwater volumes shifting from traditional mining to circular brines valorisation, thus paving the way for a resilient, "water-smart" economy, transforming industrial waste into a strategic resource for Europe.

Lectures

Lectures: Energy transition and circular economy

Analysis of hybrid energy storage systems using post-mining infrastructure, including day-ahead market (DAM) and system operating cycle characteristics.

Krzysztof Głód, Krzysztof Supernok, Agata Czardybon, Janusz Lasek [1]

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Key words: energy storage, post-mining infrastructure, day-ahead market (DAM),

The development of a new energy storage system requires an analysis of its integration with the centralised energy system. Energy production and consumption should be integrated with the day-ahead market (DAM) to optimise the cost of energy conversion. This work presents the results of an analysis of a hybrid energy storage system that uses post-mining infrastructure. The analysis took into account the day-ahead market (DAM) and the operating cycles of a pumped storage hydroelectric power station (PSH). Three types of energy storage system were analysed: CO_2 compression, air compression and traditional PSH. The optimal configuration in terms of unit profit (298 PLN/MWh) was obtained for the middle-level storage capacity system (42 MWh) in the case of the CO_2 system. Project “Hybrid energy storage system using post-mining infrastructure (HESS)” supported by Research Fund for Coal and Steel. No. 101112380 (RFCS-2022).

Aqueous organic redox flow batteries for high-temperature operation

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Environmental concerns together with gradually increasing geopolitical tensions emphasizes the need for safer and more sustainable way of securing energetic needs of growing mankind. For the aimed transition from fossil-based towards more sustainable energetics, affordable, safe and eco-friendly energy storage options are urgently needed, both for mobile and stationary applications. Redox flow batteries (RFBs) offer valuable features of decoupled power and capacity and non-flammability. Moreover, use of aqueous electrolytes also simplifies heat management and, thus, can potentially enable heat storage applications of the battery. However, with std. vanadium electrolytes, this option is typically not fully deployed due to the limited thermal stability of posolyte active species at high SOC and temperatures above 40 °C. [1, 2] Thus, alternatives active species for flow battery electrolytes are intensively sought incl. organic redox species, some of them being reported for their excellent chemical stability in a broad temperature range. [3]

In our contribution, we study chemical and electrochemical stability of the selected aqueous RFBs electrolytes using phenazine- and alloxazine-based negolytes coupled with ferrocyanide-based posolyte. The stability of the redox couples at various supporting electrolytes (pH range 7-14) was systematically evaluated in a broad temperature range (20-80 °C) for both oxidation states of active species, incl. symmetric and asymmetric flow battery single-cell testing. The post mortem analysis of the electrolyte composition using UV-vis, potentiometric titrations, HPLC and RDE measurements enabled us to identify individual mechanisms of the electrolyte degradation and to assess their contribution to the overall capacity fade observed in flow battery testing.

References:

[1] Yuan, X.-Z., *et al.*, A review of all-vanadium redox flow battery durability: Degradation mechanisms and mitigation strategies. International Journal of Energy Research, 2019. 43(13): p. 6599-6638.

[2] Choi, C., *et al.*, "A review of vanadium electrolytes for vanadium redox flow batteries," Renewable and Sustainable Energy Reviews, 2017. 69(C): p. 263-274.

[3] Xu, J., et al., "Ultrastable aqueous phenazine flow batteries with high capacity operated at elevated temperatures," Joule, 2021. 5(9): p. 2437-2449.

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Carbon Capture, Utilization and Storage (CCUS) perspectives in Indonesia and Visegrád Countries

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Abstract

As a key technology for global climate change mitigation and the pursuit of carbon neutrality, Carbon Capture, Utilization, and Storage (CCUS) is examined through a comparative analysis between Indonesia, leveraging its practical experience in the oil and gas sector and its target of 15 CCUS projects by 2030 and the Visegrád countries, which operate within the European Union's regulatory framework, including the "Fit for 55" package. Applying a socio-techno-economic approach, this study integrates the Levelized Cost of Carbon Capture (LCOCC), Social Cost of Carbon (SCC), and Levelized Cost of Electricity (LCOE) to evaluate project feasibility by calculating the Social Net Present Value (NPV Social), thereby internalizing environmental externalities. By contrasting LCOCC and SCC scenarios and incorporating the Nordhaus–Stern discount rate debate, the research identifies strategic conditions such as the need for subsidies and technological efficiency improvements under which CCUS projects can generate positive net social benefits, offering policy-relevant insights to help align technical deployment with long-term climate objectives and socio-economic sustainability in both regions.

Keywords: CCUS, LCOCC, Social Cost of Carbon (SCC), Sustainability Assessment, Indonesia, Visegrád Group.

Comparative Performance of Lithium-Ion, Sodium-Ion, and Lead-Acid Batteries in a Solar Photovoltaic System Using MATLAB/Simulink

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Key words: energy storage systems; lithium-ion batteries; sodium-ion batteries; lead-acid batteries; solar photovoltaic systems; MATLAB/Simulink simulation;

Abstract

This study analyzes the performance of lithium-ion, sodium-ion, and lead-acid batteries applied to a solar photovoltaic system using MATLAB/Simulink simulations. The evaluation considers key operational parameters, including voltage range, charging time, current behavior, and state-of-charge (SOC) evolution under identical control conditions, enabling a comparative assessment of their dynamic response when interfaced with a photovoltaic power source.

Lithium-ion batteries demonstrated the best dynamic performance, reaching full charge in approximately 3,900 s, operating within a voltage range of 80–105 V, and exhibiting stable current behavior after initial transient effects, along with a nearly linear SOC evolution. Lead-acid batteries presented a similar charging time but showed higher voltage and current fluctuations during transient operation. Sodium-ion batteries exhibited the longest charging time, a narrower voltage range, and slower SOC evolution, indicating reduced charging dynamics under the same control conditions.

Regarding thermal behavior, lithium-ion batteries require advanced thermal management strategies due to their higher susceptibility to thermal runaway. Sodium-ion batteries exhibit improved thermal stability with a reduced tendency for cascading failure, while lead-acid batteries present lower thermal runaway risk but require proper ventilation due to hydrogen gas generation during overcharging.

The results indicate that all battery technologies are technically viable when supported by appropriate power electronics and charge control strategies. However, significant differences in dynamic behavior were observed under identical operating conditions. In conclusion, lithium-ion batteries provide the most favorable overall performance for solar photovoltaic applications in terms of efficiency, stability, and dynamic response.

Quantifying the digitalisation contribution to the management of increasing RES absorption in the electricity market: the case of Slovakia

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Keywords: digitalisation, electricity market, imbalance cost, machine learning, renewable energy, price volatility

The transformation of the energy sector towards sustainable and low-carbon energy sources represents a major challenge for the stable and efficient operation of electricity systems. The increasing share of variable renewable energy sources raises the requirements for system flexibility and complicates the short-term balancing of electricity supply and demand. In this context, digitalisation technologies and advanced data-analytical tools are becoming increasingly important, as they enable more efficient processing of large volumes of data and support more accurate decision-making in energy system management. The aim of this paper is to quantify the contribution of digitalisation and advanced data-analytical tools in managing the short-term balance of the electricity system in Slovakia in the context of the ongoing transition towards sustainable energy sources. The research is based on the analysis of electricity market and power system operation data. The methodological approach includes the construction of analytical indicators, the application of predictive models, and the evaluation of their performance using statistical accuracy measures. The study also considers economic aspects derived from the results of the selected machine learning model and risk indicators such as Value at Risk (VaR), with a particular focus on their impact on imbalance costs and the functioning of balancing mechanisms. The results indicate that imbalance costs increase non-linearly with the market price level, with a fixed imbalance of 100 MWh generating costs ranging from approximately €7,500 under stable conditions to €50,000–€60,000 during stressed market periods. A stochastic analysis based on Monte Carlo simulation reveals an expected imbalance cost of approximately €19,000, while risk indicators confirm significant exposure to extreme price events. The research results in the proposal of a methodological framework that systematically links the statistical accuracy of the LightGBM model with its economic consequences in short-term electricity market environments, providing a basis for improved decision-making under conditions of increasing volatility and renewable energy penetration.

This research paper is a partial output of the project *VEGA 1/0713/24 Digital economy as a key challenge for the transformation of enterprises in Slovakia* financed by the Ministry of Education, Research, Development and Youth of the Slovak Republic.

RETROFITTING AND OPTIMIZATION STRATEGIES FOR DECARBONIZING DISTRICT HEATING SYSTEMS

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Key words: District heating, Heat pumps, Optimization

This paper investigates retrofit strategies for decarbonizing a district heating system through the integration of low-carbon technologies and optimized operation. The study focuses on the implementation of large-scale heat pumps utilizing various heat sources, including industrial waste heat, wastewater streams, and heat recovery from boiler flue gases. Thermodynamic performance of selected working fluids is evaluated using Aspen HYSYS, while system-level dispatch is analyzed using a model developed in Excel.

Realistic operating conditions are considered, including part-load behavior, electricity price driven operation, thermal storage, and hot standby modes. A condensing flue gas heat recovery system coupled with a heat pump is also assessed as an additional retrofit option. The performance of individual configurations is evaluated in terms of efficiency and contribution to heat supply.

A multi-criteria decision analysis (MCDA) framework is applied to compare the alternatives based on economic, environmental, safety and utilization criteria. Environmental evaluation includes both avoided CO_2 emissions and the impact of refrigerants, while utilization criteria reflect thermodynamic performance and annual heat supply potential. The results provide a comprehensive comparison of retrofit pathways and identify promising solutions for the transition toward low-carbon district heating systems.

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

Lectures: Bioprocess and biotechnology

Cellulose-based ionogels as novel membrane materials for microbial fuel cell applications

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Key words: cellulose ionogel, current generation, membrane separator, microbial fuel cell

Microbial fuel cells (MFC) are renewable-based energy producing electrochemical platforms. They exploit the so-called exoelectrogenic metabolism of specific bacteria. These electro-active bacteria conduct the transfer of substrate oxidation-based electrons to a conductive surface extracellularly. Such feature makes them able to be applied as waste-based energy recovery techniques. Although MFC technology has highly advantageous features in the context of renewable electricity and circular economy, the main challenges mitigating its scaled-up implementation are the cost and – more importantly – the incompatibility of the available membrane and electrode materials.

In this work, we present a novel membrane alternative based on green building blocks. Cellulose ionogels (CIg) are made by dissolving cellulose in specific ionic liquids (IL), and by a simple sol-gel transition after heat treatment. The reconstructed cellulose, thus, immobilizes IL within the formed gel phase, resulting in good ionic conductivity. CIg exhibit unique mass transport properties compared to widely used membrane materials (e.g. Nafion). To test these alternative materials as separators, experiments in MFC were conducted parallel to Nafion-MFC control. The biofilm formation stage was affected by mass transfer between the anode and cathode chambers, and the CIg membranes seemed to shorten acclimation. Comparable current density production at optimal external load was achieved, 11.9±1.9 and 9.4±1.3 A m^{-3} for Nafion-MFC and Cig-MFC, respectively. Meanwhile, internal resistance of MFCs were remarkably low (102.7±24.1 Ω and 147.2±33.7 Ω for Nafion-MFC and Cig-MFC). In summary, it turned out that CIg membranes offer a cost-effective alternative for polymeric ion exchange membrane for efficient current generation in MFC. Future research should focus on stability and manufacturing optimization of the existing and new ionogel types.

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Chromatographic Purification of Polyphenolic Compounds from a By-Product of Rapeseed Protein Isolation

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Key words: rapeseed; polyphenols; sinapic acid; chromatography; adsorption; purification

Polyphenols are an important class of plant secondary metabolites, valued for their antioxidant properties and wide-ranging applications in the food, pharmaceutical, and cosmetic industries. Rapeseed (*Brassica napus*) represents a significant source of polyphenolic compounds, particularly sinapic acid and its derivatives. During the industrial isolation of rapeseed proteins, a polyphenolic-rich by-product is generated, offering an opportunity for further valorization.

The aim of this work was to investigate the efficacy of chromatographic techniques for the purification of polyphenolic compounds from this by-product. The study focused on adsorption-based separation using a non-polar polymeric adsorbent, with a specific emphasis on how key process parameters, namely pH and column loading, influence separation efficiency.

The adsorption behavior of the target polyphenolic compounds was evaluated under varying conditions, and chromatographic experiments were carried out to assess the feasibility of their separation from complex mixtures. Our results indicate that separation efficiency is governed by both the physicochemical properties of the target compounds and operating conditions. The distinct elution profiles observed for individual polyphenols demonstrate the potential for selective purification through the optimization of process parameters.

Overall, these findings confirm that chromatographic purification is a promising approach for the recovery of valuable polyphenolic compounds from rapeseed processing by-products. This strategy supports the sustainable utilization of agro-industrial residues and facilitates the development of high-value functional ingredients. Future research should focus on further process optimization and considerations for industrial scale-up.

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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: Baeyer-Villiger oxidation; enzymatic cascade; whole-cell biocatalyst; lactones

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 comprising alcohol dehydrogenase (ADH), enoate reductase (ER), and cyclohexanone monoxygenase (CHMO) that efficiently converts 2-cyclohexen-1-ol to ε-caprolactone.

We investigated the effect of oxygen transfer coefficient (k_La) and cell concentration (c_X) on the efficiency of oxidation of cyclohexanone to ε-caprolactone. The results indicated that the product formation rate was strongly dependent on the optimal setting of k_La in relation to c_X, due to the simultaneous consumption of oxygen by BVO and cell metabolism.

We further studied the effect of ethanol as an inhibitor of ADH, which catalyzes not only the first cascade step 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.

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Evaluating microbial desalination kinetics and efficiency at various substrate loadings and initial salinity

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Key words: electrochemical desalination, microbial desalination cell, acetate, ion exchange membrane, current efficiency

Abstract

The importance of desalination technologies and research is increasing every year, as a significant number of countries do not have adequate drinking water supplies or their distribution does not allow for sufficient supply. By reducing the salt concentration of sea and brackish waters (e.g. using reverse osmosis), it is possible to produce water suitable for consumption and agricultural usage. Nowadays more research is being published that uses bioelectrochemical systems (BES) for desalination, especially microbial desalination cells (MDC).

In this study, a comparative evaluation of the effect of different substrate and initial NaCl concentration on the desalination kinetics and efficiency is presented. In addition, the membrane-related voltage losses in MDC are analysed. The mesurements with the three different substrate concentration (C_{Ac}= 2.5, 5.0 and 7.5mM acetate) resulted in different desalination efficiency with 35 gL^{-1} NaCl solution using mixed culture three-chamber MDC. The higher loading of acetate resulted in higher current density, but the current generation kinetics was inversely proportional to C_{Ac}. Evaluating the effect of the initial NaCl concentration (15, 20, 25 and 35 gL^{-1}) on the MDC performance showed that it determined the desalination kinetics significantly only at the early stage of the operation. Initial salinity had a significant effect on the NaCl removal during the 24 h batch cycles. At 35 gL^{-1}, up to 42 % removal could be achieved compared to ~ 27 % in case of C_{NaCl}=15 gL^{-1}. Meanwhile, final desalination rates were independent of C_{NaCl}. Current efficiencies decreased from 40-100% to 20-35% during the operational cycle. Resistance and loss analysis revealed that mass transfer resistance was the dominating factor of MDC operation, and at low C_{NaCl}=15 gL^{-1} more severe concentration polarization occurred.

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Hydrogel Microactuators for Laser-Induced Mechanical Stimulation in 3D Cell Culture

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Key words: hydrogel microactuators; mechanical stimulation; 3D cell culture; stop-flow lithography; photocrosslinkable hydrogels

Cells in living tissues are continuously exposed to mechanical stimuli that regulate their morphology, migration, and biochemical signaling. However, delivering localized and well-controlled mechanical stimulation to cells embedded in soft three-dimensional (3D) matrices remains challenging for in vitro studies. Most current approaches rely on bulk deformation of hydrogels or macroscopic mechanical loading, limiting spatial precision and control of applied forces. To address these limitations, we developed a soft hydrogel-based microactuator capable of generating controllable mechanical stimulation directly within 3D cell culture environments.
The microactuator is fabricated using stop-flow lithography in microfluidic channels and consists of a composite hydrogel structure. A passive polyethylene glycol diacrylate (PEGDA) backbone is combined with a thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) segment doped with gold nanoparticles. Upon green laser irradiation (532 nm), localized plasmonic heating induces reversible contraction of the active segment, generating deformation of a central hydrogel bridge containing encapsulated cells.
Several photocrosslinkable hydrogels (Dex-HEMA, HAMA, ColMA, and methacrylated human platelet lysate – hPLMA) were evaluated as matrices for cell encapsulation using anterior cruciate ligament fibroblasts. Most hydrogels maintained cell viability above 80 % after seven days of culture. Protein-based hydrogels supported favorable cell morphology, while Dex-HEMA constructs showed depth-dependent viability due to diffusion limitations. Based on biocompatibility and fabrication compatibility, hPLMA was selected as the most suitable hydrogel for integration into the actuator system.
The developed platform enables reversible and tunable mechanical stimulation with forces in the micronewton range and stable cyclic actuation. This system provides a versatile tool for studying mechanobiological responses of cells in soft 3D microenvironments.

Preparative chromatographic separation of polyphenols from black chokeberry and sea buckthorn with macroporous resins

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Key words: polyphenols, chromatographic separation, macroporous resins, berries, antioxidants

The rising global awareness of health and nutrition has driven a significant increase in demand for functional foods that offer bioactive benefits. Polyphenols have gained popularity due to their antioxidant, anticancer, neuroprotective, and antidiabetic properties. This study investigates black chokeberry and sea buckthorn, fruits rich in these compounds but currently underutilized due to their astringency and acidity. To address this, we developed a systematic approach for the extraction and purification of these high-value compounds.

Initial experiments focused on preparing ethanol extracts and identifying primary bioactive compounds: seven compounds in black chokeberry and four in sea buckthorn. To optimize purification, a comprehensive screening of 26 adsorbents was conducted. Based on kinetic and adsorption isotherm experiments, the three most efficient resins—PAD600, FPX66, and XAD1180N—were selected for preparative column chromatography (d = 1 cm, L = 10 cm). Separations were performed using a controlled step gradient of ethanol to isolate compounds based on their relative polarities.

Results demonstrated that PAD600 was the most effective for recovering phenolic acids from black chokeberry. Conversely, XAD1180N proved superior for anthocyanin separation, achieving a 62% yield of cyanidin 3-glucoside in the 20% ethanol fraction, while also excelling in the isolation of the less polar rutin and quercetin 3-glucoside. In sea buckthorn separation, the highly polar vitamin C eluted probably primarily during the initial sample loading. Medium-polarity quercetin and isorhamnetin glycosides were concentrated in the 20% ethanol fraction, with recovery yields increasing in the order of PAD600 < FPX66 < XAD1180N.

These findings provide a systematic framework for the selective isolation of high-purity polyphenols, offering a viable pathway for transforming underutilized agricultural products into valuable ingredients for the nutraceutical industry. Furthermore, this approach supports the circular economy by repurposing industrial waste into high-value commodities, thereby increasing crop profitability while making their delivering potent health benefits in a palatable, concentrated format.

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Small-scale bioreactors: challenges in experimental determination of hydrodynamic stress in stirred vessels

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Key words: small-scale bioreactors, maximum hydrodynamic stress, shear-stress-sensitive aggregates, particle image analysis, optical microscopy

The rapid development of human mesenchymal stem cell (MSCs)-based cell therapies creates a strong demand for scalable, controlled, and reproducible manufacturing processes capable of delivering clinically relevant cell numbers. Bioreactor systems fulfill these requirements, however there is the need for efficient bioprocess design and optimization. During such cultivation, MSCs are exposed to complex hydrodynamic forces generated by mixing and aeration. Although adequate mixing is essential for efficient heat and mass transfer, maximum hydrodynamic stress (τ_{max}) can affect cell viability and productivity. Direct evaluation of these effects using cell-based culture experiments is both time-consuming and inefficient, highlighting the need for alternative approaches to characterise τ_{max} in bioreactor systems.
In this study, shear-stress-sensitive aggregates, based on polymethylmethacrylate nanoparticles, were used as low-cost universal probes for τ_{max} characterisation in stirred bioreactors. Conventionally, aggregate size is determined by static light scattering (SLS); however, this approach requires relatively large sampling volumes, which limits its applicability in small-scale bioreactor systems and results in discontinuous and time-intensive analysis. To address these limitations, we developed and implemented a low-volume analytical approach based on optical microscopy image analysis for aggregate size determination. An optical flow-through cell was designed to allow continuous sampling and was tested using the high-throughput ambr®250 mL bioreactor system equipped with multiple impeller configurations. The comparative analysis demonstrated strong agreement between microscopy-based measurements and conventional SLS results, indicating that the proposed method can fully substitute SLS for τ_{max} characterisation. In addition, the approach enables continuous monitoring of particle size while reducing the sampling volume by approximately one order of magnitude.
The presented method provides an effective tool for real-time in situ characterisation of τ_{max} in bioreactor systems. Improved quantification of hydrodynamic forces in stirred and aerated bioreactors will support more reliable scale-up and scale-down strategies and contribute to enhanced reproducibility and standardisation of MSCs cultivation processes.

Spray-dried bioactive microparticles for antimicrobial applications

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Key words: spray drying, microparticles, allicin, inclusion complexes, antimicrobial activity

Achieving a controlled antimicrobial effect with unstable bioactive compounds remains a major limitation of delivery strategies, particularly when evaluated against highly adaptable pathogens. *Pseudomonas aeruginosa* represents a challenging model system as its metabolic flexibility and tolerance mechanisms allow it to maintain growth even under inhibitory conditions. Among the substances that could overcome this tolerance, allicin has attracted attention due to its broad-spectrum antimicrobial activity. However, its application is limited by chemical instability, which complicates its formulation and controlled release. Particle-based systems have therefore been developed that enable the formation of allicin *in situ* from separately encapsulated alliin and alliinase, with the aim of mimicking its natural formation and increasing its stability. Although this approach is effective, it relies on enzymatic activation, which introduces variability and limits precise control over the final dose. Building on these limitations, two complementary delivery strategies are explored. The first approach retains the established concept of enzymatic *in situ* formation using lactose–leucine microparticles containing separately encapsulated alliin and alliinase. The second strategy replaces enzymatic activation by direct incorporation of pre-synthesized allicin, stabilized through inclusion complexation with β-cyclodextrin and formulated into lactose–β-cyclodextrin–leucine microparticles via spray drying. The formulations are evaluated for aerodynamic behaviour and antimicrobial efficacy by tracking growth dynamics of *Pseudomonas aeruginosa* PA01. Preliminary results suggest comparable antimicrobial effects for both approaches, indicating that direct delivery of stabilized allicin may provide an alternative to enzymatic *in situ* formation while allowing control over formulation design.

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The 2-phenylacetic acid derivatives functionalized with $–NH_2$ and $-NO_2$ groups: FMO, NBO, UV-Vis, Pharmacokinetics studies

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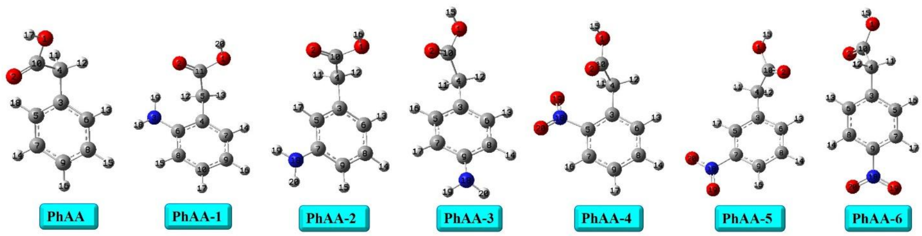
The phenyl-acetic acid (PAA), known as a natural auxin, is sourced mostly from fruits and has antimicrobial, antioxidant, and antifungal activities. Herein, the -NH2 and -NO2 groups were used to functionalize the PAA core structure, changing the positions of these groups. The effect on the reactivity, electronic spectra, and pharmacokinetics profiles of the substituent group and position on the PAA was investigated using computational tools. The geometry optimizations of the compounds were conducted at B3LYP/6-311++G** level, and then each of the structures was confirmed by no negative frequencies. The TD-DFT simulations were performed to elucidate the electronic spectra of the compounds. The NBO simulations were conducted to estimate and then evaluate the intramolecular interactions that contribute to decreasing stabilization energy. The FMO and MEP analyses were also performed to determine the global reactivity features and reactive site(s) of the compounds. The pharmacokinetics, drug-likeness, and bioavailability indexes were predicted using SwissADME tools.



Key Words: *phenylacetic acid, UV-Vis, FMO, NBO, MEP, pharmacokinetics*

Acknowledgement: All calculations have been conducted at TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). The author thanks the Scientific Research Projects Department of Cumhuriyet University (Project No: EĞT-2023-098).

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The substitution group and solvent effect on the chemical behavior of chlorine-functionalized Ferulic acid

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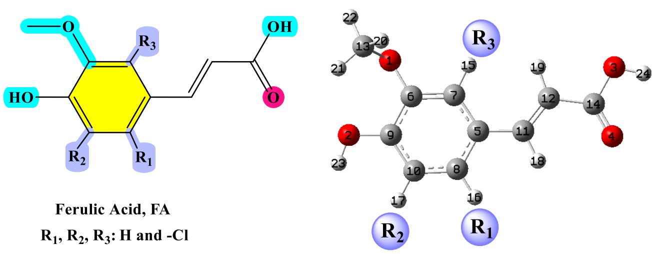
Ferulic acid (FA) as a member of the phenolic compounds have occurred in the plants commonly, especially in popocorns, bamboo shoots, rice, and wheat [1]. Also, it is the main metabolite of the chlorogenic acids in humans together with caffeic and isoferulic acid. G16W package [2] is used to perform the quantum mechanical simulations. Herein, the DFT/B3LYP/6-311++G** [3,4] level computations are conducted to structural optimization and confirmation of the FA and its chlorinated derivatives depicted in Figure 1. Then, the FMO and MEP computations are performed to elucidate the reactivity direction [5] and site of the compounds. Also, the TD-DFT computations have been conducted to evaluate the UV-Vis characterization. The pharmacokinetics, bioavailability, and drug-likeness features of the compounds are also evaluated [6].



Key Words: *Ferulic acid, UV-Vis, FMO, NBO, MEP*

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Lectures: Risk management and process safety

Dynamic Modelling Approach to Identifying Critical Operating Conditions in Ammonia Synthesis

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Key words: Ammonia, Simulation, HAZOP

This work deals with ammonia as one of the main products of the global chemical industry. The nonlinear character of the ammonia synthesis process is studied, with a focus on analysing how the system responds to changes in operating parameters. Ammonia synthesis is a highly exothermic reaction, which can be dangerous under abnormal operating conditions. In this work, sensitivity analysis is carried out under both steady-state and dynamic conditions to evaluate process stability and to identify regions where unstable or unpredictable behaviour may occur. The Morris method is used to determine how individual input parameters affect the process and to identify the most important ones. A systematic identification of potentially hazardous operating states is performed using the HAZOP methodology, which is adapted for evaluating results from numerical simulations. The response of the ammonia synthesis loop to changes in selected process parameters within given ranges is also investigated. A steady-state simulation of the process is created in Aspen Plus, while a dynamic model is developed in Aspen Plus Dynamics to study how the process behaves over time under disturbances. The results show that combining dynamic modelling with sensitivity analysis is a useful approach for improving process safety and better understanding the behaviour of the system.

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Influence of collision velocity on triboelectric charging of polyolefin particles

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Key words: triboelectric charging, polyolefins, surface roughness, collision velocity

The triboelectric charging of electrically insulative particles causes operational problems in many industrial processes. For example, it causes unwanted particle adhesion to reactor walls during the production of polyolefins in gas-phase fluidized beds, which leads to the formation of wall sheets and reactor shutdown. The underlying mechanism of triboelectric charging is, however, not fully understood, and current mathematical models based on Discrete Element Method (DEM) have several limitations. These include: (i) the models neglect particle surface roughness; (ii) the large computational cost of DEM simulations. Therefore, we developed a DEM particle-wall collision model that includes particle surface roughness, and we then focused on reducing the computational time. Particles were geometrically described as smooth spherical cores with semi-spherical asperities on their surfaces. Existing contact mechanics models were then modified to include the effects of this surface roughness. Saturation charges were evaluated based on particle size, material properties, surface roughness, and collision velocity. Our results show that surface roughness has an important effect: saturation charge is a function of collision velocity. This is supported by experimental data and cannot be explained by models that neglect surface roughness. Moreover, based on the results of model parametric studies, we show that assuming all surface asperities have the same height, a single function of all input parameters can be used as a surrogate model, thus significantly reducing the computational time.

Lectures: Environmental chemical engineering

Application of Natural Deep Eutectic Solvents for the Extraction of Bioactive Compounds from Rapeseed Meal

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Key words: Rapeseed meal, Deep eutectic solvents, Ultrasound-assisted extraction, phenolic antioxidants, Green extraction

Rapeseed meal, an abundant by-product of the oil industry, is a promising source of natural antioxidant compounds. This study investigated ultrasound-assisted extraction using choline chloride-based deep eutectic solvents as a greener alternative to conventional organic solvents for recovering valuable bioactive constituents from rapeseed meal. Different solvent formulations were examined, and the choline chloride/urea system showed the greatest extraction effectiveness. To further improve the process, response surface methodology with a Box–Behnken design was used to evaluate the influence of extraction temperature, time, and solvent to DES ratio on extract quality. The recovered extracts were assessed for their overall antioxidant potential and total phenolic content. Under optimized conditions, the extraction process yielded extracts with strong antioxidant properties, and the experimental findings closely matched the model predictions. In comparison with conventional methanolic extraction, the deep eutectic solvent-based ultrasound approach proved to be both efficient and more environmentally sustainable for the recovery of antioxidant compounds from rapeseed meal. These results underline the potential of deep eutectic solvents as green extraction media for the valorization of oilseed processing by-products.

Combined Physicochemical Processes for Quaternary Wastewater Treatment

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Key words: coagulation, ozonation, sand filtration, quaternary treatment, wastewater reuse

This study investigates the effectiveness of combined coagulation, sand filtration, and ozonation for advanced treatment of wastewater effluent from a municipal wastewater treatment plant. Coagulation using $FeCl_3$ followed by sand filtration served as a pre-treatment step prior to ozonation. This approach proved to be essential not only for partial pollutant removal but also for enhancing the efficiency of subsequent ozonation. The pre-treatment significantly improved water quality, achieving a 51% reduction in COD_{Cr} (from 21.8 to 10.67 mg/L), a decrease in total nitrogen from 35.9 to 30.5 mg/L. Total phosphorus was effectively removed to below the detection limit (<0.033 mg/L), essentially confirming the high efficiency of phosphorus precipitation by inorganic salts. In addition to chemical parameters, a significant reduction in microbial contamination was observed. Coliform bacteria and *Escherichia coli* were reduced by approximately two orders of magnitude, while thermotolerant coliform bacteria and intestinal *Enterococci* decreased by up to three orders of magnitude after coagulation and filtration. Ozonation was applied at different generator outputs (20%, 40%, and 60%), with relatively small differences in removal efficiency between the tested conditions. However, pre-treated samples consistently showed higher pollutant removal compared to untreated wastewater. Ozonation of raw effluent resulted in minimal improvements in COD_{Cr} and nitrogen removal, highlighting the importance of pre-treatment. Complete microbial inactivation was achieved after ozonation, demonstrating its strong disinfection capability without the addition of residual chemicals. Kinetic analysis of COD_{Cr} degradation indicated that the process does not follow zero-order kinetics. Instead, a second-order kinetic model provided the best fit with coefficient of determination $R^2 = 0.9328$, suggesting a non-linear reaction mechanism. Overall, the combined application of coagulation, sand filtration, and ozonation represents an effective quaternary treatment strategy, significantly improving physicochemical and microbiological water quality and supporting the safe reuse of treated wastewater.

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Energy assessment of brine processing

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Keywords: Industrial brines, Energy consumption, Heat pump, Membrane distillation.

The recovery of valuable materials from industrial brines represents a key strategy in advancing the circular economy. However, these processes are traditionally associated with high energy intensity due to the substantial heat requirements for evaporation and crystallization. This study presents a model-based comparative assessment of various energy integrations aimed at improving energy efficiency and reducing the overall environmental footprint of brine treatment. The research utilizes Aspen Plus software to simulate and evaluate several configurations. A multi-effect evaporator serves as the baseline design, which is compared against newer integrated systems featuring electric heat pumps, thermocompressors, and hybrid arrangements based on membrane distillation. The study focuses on evaluating how different heat integration technologies influence both the thermal performance and the economic viability of the recovery process. The results showed that integrating these new technologies brings major improvements. Using heat pumps and thermocompressors significantly reduced the need for external heating steam by successfully recycling energy within the system. The best economic results were achieved by the systems using membrane distillation, which proved to be the most cost-effective option overall. Furthermore, the study found that the specific type of salt being processed greatly affects the efficiency.. Overall, upgrading traditional evaporation systems with these integrated technologies is a highly effective and simple way to save energy and lower the costs of industrial brine treatment.

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Zinc Speciation in Dust from a Secondary Dedusting System of the Basic Oxygen Furnace

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Key words: Secondary BOF dust; zinc speciation; sequential extraction

Abstract

Dusts generated in secondary dedusting systems of basic oxygen furnace (BOF) steelmaking constitute fine-grained, iron-bearing residues with elevated zinc contents that limit their internal recycling potential in integrated steel mills. While the chemical form of zinc in dusts from primary BOF dedusting systems has been extensively investigated, comparable information for secondary BOF dusts remains scarce. In the present study, dust collected from a secondary BOF dedusting fabric filter was comprehensively characterized with respect to particle size distribution, morphology, elemental composition, and zinc speciation. Particle size analysis revealed a broad distribution with a median particle diameter of 22 µm, consistent with reported values for secondary BOF dusts. Scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy demonstrated pronounced surface enrichment of zinc, attributed to condensation of volatilized zinc species during rapid off-gas cooling. The total zinc content of the dust was 133 g/kg. Zinc speciation was determined using a five-step sequential extraction procedure supported by X-ray diffraction analysis. More than half of the zinc (54%) was associated with oxide phases, predominantly zinc oxide, whereas zinc ferrite ($ZnFe2O4$) represented only a minor fraction. Compared to primary BOF dusts, secondary dedusting dusts exhibit a significantly higher proportion of readily leachable zinc species. These findings indicate an enhanced suitability of secondary BOF dusts for hydrometallurgical zinc removal, thereby supporting improved recycling strategies and reduced landfill disposal in integrated steelmaking operations.

Lectures: Process design and process intensification

Alignment of characteristic times in microfluidic systems for the preparation of enantiomers

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Our contribution addresses the design of microfluidic systems with harmonized characteristic times for the continuous synthesis and separation of chiral chemicals. The concept is based on matching the residence times of individual modules in modular microfluidic arrangements to achieve time-balanced reaction and separation processes. Two case studies are presented: the enzymatic production of mandelic acid enantiomers and the synthesis of (*R*)-1-phenylethanol. In both systems, immobilized lipases are used in packed-bed microreactors to perform enantioselective biocatalytic transformations. The reaction products are subsequently separated using orthogonal techniques such as electrically driven membrane separation or microfluidic liquid–liquid extraction. Harmonization of characteristic transport times, including convection and electromigration, enables efficient coupling of synthesis and separation in continuous flow. The results demonstrate that proper matching of characteristic times allows individual modules to operate with comparable volumes and performance.

Keywords: enantiomer; mandelic acid; (*R*)-1-phenylethanol; orthogonal separation; continuous flow separation

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Application of GPU-Based Computation in Chemical and Safety Engineering

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Keywords: GPU acceleration; vapor-liquid equilibrium; reaction-diffusion systems; CSTR modeling; global sensitivity analysis; numerical methods

The work is focused on investigation of the possibilities of using GPU-accelerated computations in chemical and safety engineering, with an emphasis on evaluating their practical applicability for solving computationally demanding problems and on comparing different approaches to parallelization. The study considers implementations in MATLAB using the Parallel Computing Toolbox as well as lower-level approaches based on the ILGPU library in C#.

As a first part of the solution, a mathematical model describing vapor-liquid equilibrium (VLE) for a binary ethanol-benzene system was developed. The model is based on a modified Raoult's law combined with the NRTL activity coefficient model and requires repeated numerical solution of a nonlinear equation for equilibrium temperature. Due to the large number of independent evaluations, the problem was suitable for parallelization. Sequential, vectorized, and GPU-based implementations were created and compared. The results showed that GPU acceleration provides a significant reduction in computation time, achieving a speed-up of up to 140× times, compared to the sequential CPU implementation.

In the second part, a custom numerical solver for systems of ordinary differential equations based on an adaptive Runge-Kutta method was developed and applied to a dynamic model of a continuous stirred tank reactor (CSTR). The model including reaction kinetics, heat balances and mass balances, was used to perform large sets of independent simulations with randomly generated input parameters. These simulations were further analyzed using Monte Carlo methods and the Morris method for global sensitivity analysis. In this case, GPU acceleration enabled efficient processing large number of simulations, achieving a 74× times speed-up compared to sequential implementation.

Third part of the work focused on a two-dimensional reaction-diffusion model describing the coupled transport of chemical species and heat with an exothermic reaction. The model is formulated as a system of nonlinear partial differential equations and solved using an explicit finite difference method on a spatial grid. In contrast with previous cases, parallelization was applied within a single simulation by distributing computations across spatial grid points. The results demonstrated that this type of data-parallel problem is also suited for GPU acceleration, with a speed-up of approximately 26×.

The obtained results indicate that GPU-based approaches can significantly reduce computational time across a wide range of problems in chemical and safety engineering.

Make-up water production from laboratory-scale experiments and industrial-scale design

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Keywords: make-up water, membrane filtration, coagulation, hydraulic resistance, Danube water, pretreatment

Growing global energy demand and the water-quality requirements for thermal power plant operations necessitate a reliable, scalable method for producing pure water as make-up. Two stages were investigated during this work for the Danube River water treatment. First, a pretreatment comparison of different methods for the removal of organic carbon and suspended solids, followed by a pressure-driven membrane filtration sequence with the goal of choosing appropriate flux and flow rates, for different working pressures.

In the pretreatment study, a hybrid process of coagulation followed by microfiltration, using jar tests, was followed by dead-end filtration through a 0.45 µm membrane. Prior to coagulation, the disinfection effect was tested. Ferric chloride ($FeCl_3$) and poly-aluminium chloride (PACl) were tested across a range of concentrations. $FeCl_3$ consistently outperformed PACl, achieving up to 78% total suspended solids removal and approximately 62% reduction in total organic carbon content at a concentration of 33.3 mg/L without pre-disinfection. Disinfection proved counterproductive, decreasing TOC removal efficiency, as the formation of disinfection byproducts (DBPs) reduced organic carbon removal efficiency by up to 27%.

Using a pressure-driven filtration sequence comprising ultrafiltration, nanofiltration, and reverse osmosis, the analysis of varying transmembrane pressure was conducted for each membrane. The constant-pressure operation confirmed a linear operating regime for each membrane, enabling the estimation of a resistance factor suitable for pump sizing and system design. The parameters derived from the bench experiments were then scaled up to an industrial system to produce 26.1 m^3/h of pure water suitable as make-up water for a thermal power plant.

The findings demonstrate that combining hybrid methods, using a coagulation-assisted pretreatment step based on $FeCl_3$, shows that minimal chemical use, coupled with microfiltration, provides a good starting point for the following membrane sequence and an industrial-scale blueprint for make-up water production in thermal power plants.

Lectures: Digitalization and process control

Multi-Emissivity Measurement Device for Monitoring and Control of Radiative Heating Systems

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Key words: radiative heating systems, radiative heat flux, convective heat transfer, process monitoring, multi-emissivity targets, heat transfer measurement

Radiative heating systems are widely applied in industrial buildings due to their ability to deliver heat efficiently over long distances without heating the entire air volume. In practice, however, system performance is usually assessed only from air temperature or surface temperature, while the incident radiative heat flux is not measured directly. This reduces the reliability of predicting the thermal response of heated objects. As a consequence, heating control may be inaccurate, resulting in increased energy consumption and deviations from the desired temperature conditions. Although instruments for direct measurement of radiative heat flux already exist, their high cost makes large-scale installation in industrial applications economically impractical. To address this limitation, a multi-emissivity measurement device for monitoring and control of radiative heating systems was developed and experimentally validated. The proposed device consists of four aluminium targets with different surface emissivities in the range of 0.05 to 0.94. The rear side of each target is thermally insulated, while the front side is exposed to a radiative heat source. During the experiment, the temperatures of the targets and the surrounding air are continuously recorded. The incident radiative heat flux and the convective heat transfer coefficient are determined from the transient energy balance of each target. By combining the responses of targets with different emissivities, a system of independent equations is obtained, enabling simultaneous evaluation of both unknown parameters from the measured temperature curves. The experimental results confirmed the expected emissivity-dependent heating behaviour of the targets, whereas the surrounding air temperature remained nearly constant during the measurement. For the investigated configuration, the evaluated radiative heat flux was 195 $W \cdot m^{-2}$ and the convective heat transfer coefficient was 6.5 $W \cdot m^{-2} \cdot K^{-1}$, corresponding to the typical range of natural convection in indoor environments. The calculated radiative heat flux differed by approximately 6% from the theoretical model of the source under identical geometric conditions. Compared with conventional radiometric methods, the proposed approach enables separation of radiative and convective heat transfer components without the use of expensive radiometers. The developed device therefore represents a promising low-cost tool for measurement, monitoring, and future control of radiative heating systems in industrial applications.

Lectures: Separation processes and transport phenomena

DETERMINATION OF SORPTION SELECTIVITY IN ION EXCHANGE MEMBRANES AND ITS INFLUENCE ON ION TRANSPORT

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Key words: Donnan dialysis, ion exchange membranes, ion exchange equilibria

The ion exchange membranes are a type of membrane containing a charged groups fixed on the polymer matrix, composing the membrane, which allows them to selectively transport ions based on their ionic charge. These membranes are utilized in a variety of different processes, called an electromembrane processes. These processes are becoming of an increasing interest due to their ability to separate ions from solutions. This can be utilized in a several applications for separating ions from a variety of different streams, especially waste streams. The examples of these processes include the recovery of heavy meatal ions from wastewaters or utilization of salts present in the desalination brines. The ion exchange membranes used in these applications are characterized by a variety of different parameters. These parameters include their structural properties, such as density or porosity, as well as their sorption properties. The sorption properties include the parameters such as concentration of fixed charge groups present in the membrane structure, selectivity between the ions of different charges or selectivity for ions of the same charge. The objective of this study was the experimental determination of these key sorption parameters, for a anion exchange membrane. These parameters were determined in a series of sorption experiments for a binary mixture of four different anions. In addition to the experimental determination of these sorption parameters an approach for prediction of the sorption selectivity for a different binary mixture is discussed and verified, together with example of importance of the sorption selectivity on ion transport through membrane. The results show the importance of the sorption selectivity as well as its impact on the electromembrane processes, as demonstrated in this work using the example of Donnan dialysis.

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Effect of non-ionic surfactants on velocity of single rising bubble

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Key words: bubble velocity, interphase mobility, non-ionic surfactant

Surface-active agents are essential components in numerous industrial multiphase processes, where they significantly alter the properties of phase interfaces. The present study investigates the influence of non-ionic surfactants on the behavior of an isolated bubble rising in a stationary liquid. This simple type of experiment is ideal to monitor changes in bubble velocity, which is a key parameter for determining bubble surface mobility and its degree of contamination. Uneven surfactant distribution generates Marangoni stresses, increasing the drag coefficient (Manikantan, 2020). Five non-ionic surfactants (n-propanol, n-pentanol, n-octanol, α-Terpineol, Triton X-100) differing in their molecular structure and adsorption/diffusion dynamics at the gas-liquid interface are examined. A wide range of surfactant concentrations was tested, and adsorption/diffusion dynamics were evaluated using equilibrium and dynamic surface tension measurements.
The results demonstrate that the degree of surface immobilization and the resulting reduction in bubble velocity strongly correlate with the surfactant's molecular structure and adsorption kinetics. A significant contrast was observed between short-chain alcohols and large surfactant molecules; for instance, Triton X-100 induced complete surface immobilization at concentrations six orders of magnitude lower than those required for n-propanol. Furthermore, local velocity profiles revealed different rates of surface loading. The study provides a comprehensive overview of the influence of the absorption kinetics of nonionic surfactants on bubble behavior.

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Electrodialytic separation of bio-based volatile fatty acids (C2-C6)

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Keywords: waste valorisation, acidogenic fermentation, carboxylic acid separation, electrodialysis, bipolar membrane

Volatile fatty acids (VFAs) produced during the bioconversion of organic substrates (such as biowaste) have attracted increasing attention due to their broad applicability as platform chemicals, precursors for bio-based products, and intermediates in circular biorefinery concepts. However, their efficient recovery from complex fermentation broths are still challanging and limited. Electrodialysis (ED) represents a promising separation technology for this purpose, as it enables the selective transport and concentration of ionizable components under an applied electric field. In this study, real fermentation effluents were treated using an electrodialysis system to investigate the separation kinetic and recovery of organic acids. The energy consumptions were between 0.26-0.32 kwh/kg VFA, and the product recovery values regarding the short-chain acids (C2-C4) were between 80-95%. These findings support the potential application of electrodialysis as a downstream processing step in VFA-based bioconversion and waste valorisation systems.

Free-Flow Electrophoresis: An experimental platform for continuous separation of enantiomers

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Optically active compounds are widely used as active pharmaceutical ingredients (APIs) or as precursors in drug manufacturing. Therefore, the pharmaceutical industry places strong emphasis on the production of optically pure and enantiomerically enriched compounds. Traditionally, these are obtained through asymmetric synthesis or chromatographic methods, which are often time-consuming, expensive, and unsuitable for continuous operation. Alternatives include enantioselective enzymatic reactions catalyzed by lipases in packed-bed reactors or the separation of enantiomers from racemic mixtures using orthogonal techniques.

Microfluidic technologies and orthogonal separation methods, particularly free-flow electrophoresis (FFE), represent promising approaches for continuous separations. FFE enables fractionation of electrically charged compounds based on differences in electrophoretic mobility. However, its broader application is still limited by lower separation efficiency compared to conventional techniques such as chromatography. Further development therefore requires a deeper understanding of transport phenomena, including interactions between analytes, electrolyte components, and the applied electric field.

In this work, we focused on the separation of mandelic acid enantiomers using a chiral selector dissolved in the electrolyte. A positively charged β-cyclodextrin derivative was used, which preferentially binds to one enantiomer and alters its electrophoretic mobility. Partial enantiomer separation was experimentally demonstrated, indicating the potential of FFE for continuous separation of optically active compounds.

Building on these results, we further develop a concept employing superparamagnetic iron oxide nanoparticles (SPIONs) as mobile carriers of chiral selectors. The nanoparticle surface can be chemically modified to control both ligand attachment and surface charge. Functionalized particles are deflected in the electric field to intersect the racemic stream, enabling selective binding of one enantiomer and its diversion into a different trajectory, while the other continues unaffected. This controlled trajectory crossing represents a promising strategy to enhance the efficiency of continuous enantioseparation in FFE systems.

Publications:

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Selective Sorption of CO_2 and SO_2 in PEEK–Ionene Composite Membranes for Flue Gas Treatment

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This study integrates an innovative experimental sorption methodology with conventional Grand Canonical Monte Carlo (GCMC) and molecular dynamics (MD) simulations to deepen the understanding of gas sorption phenomena in materials developed for CO_2 and SO_2 removal from industrial flue gases. The advancement of efficient purification technologies for sour gas removal critically depends on the rational design of advanced materials and detailed insight into their physicochemical behavior.

Experimental measurements and molecular modeling were employed to investigate the sorption behavior of sour gases (CO_2 and SO_2), a sweet gas (CH_4), and SO_2/N_2 mixtures in advanced poly(ether ether ketone) (PEEK)–ionene composite membranes. These materials consist of PEEK backbones interconnected with imidazolium groups, featuring variations in imidazolium structure and different loadings of incorporated ionic liquids (ILs). The influence of both the imidazolium moiety and IL content on gas sorption performance was systematically evaluated.

The results demonstrate that SO_2 exhibits the highest sorption affinity, even at low concentrations (~5000 ppm) in N_2-rich mixtures. The sorption selectivity follows the order:

$\mathbf{SO_2 > CO_2 > CH_4 > N_2}$

A PEEK–ionene variant lacking a methyl substituent on the imidazolium ring displayed enhanced CO_2/N_2 solubility selectivity compared to its methyl-substituted counterpart. However, increasing pressure reduced this selectivity difference by approximately fivefold. This behavior is attributed to restricted polymer chain mobility at elevated pressures, resulting in a dominant contribution of the free IL phase to gas transport within the composite membrane.

Molecular simulations further revealed that the polymer end-to-end distance reaches a maximum at an IL loading of two equivalents. Higher IL contents induce polymer chain contraction, accompanied by a decrease in polymer density. These findings provide valuable insight into the structure–property relationships governing gas sorption in PEEK–ionene composite membranes and support their promising application in flue gas purification.

Acknowledgments

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Investigation of the vapor-liquid phase equilibrium of a binary mixture of eucalyptol and various alcohols

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Keywords: alcohols, vapor liquid equilibrium, theoretical and computational chemistry

The development and selection of alternative, sustainable solvents have become a key focus in modern chemical engineering, driven by the need to replace volatile, toxic, and fossil-based organic solvents.[1] In this context, naturally derived compounds such as eucalyptol have gained increasing attention due to their favorable environmental and safety profiles.[2] However, the practical application of such solvents requires a thorough understanding of their thermodynamic behavior, particularly in mixtures with common polar solvents such as short-chain alcohols.

The aim of this work was to investigate the thermodynamic and separation behavior of binary liquid mixtures, specifically those composed of eucalyptol and three alcohols: methanol, ethanol, and n-propanol. Various activity coefficient models (Wilson, UNIQUAC, NRTL, UNIFAC) were applied to describe the interactions between components and to evaluate the applicability of each model for these systems.

Experimental measurements were performed at atmospheric pressure, covering a wide concentration range. The data, based on refractive index measurements, were processed using regression methods to fit the different thermodynamic models, and the binary interaction parameters required for vapor–liquid equilibrium calculations were determined.

In the case of the methanol–eucalyptol mixture, the UNIQUAC model showed the best fit for temperature data, while the Wilson model gave the most accurate results for the y_1 values. For the ethanol–eucalyptol system, the Wilson model matched the temperature trends more closely, whereas the NRTL model provided more accurate composition predictions. For the n-propanol mixture, the Wilson model again performed best in terms of temperature, while the UNIQUAC model gave better results for y_1.

Notable differences were observed among the applied models. In the case of the methanol–eucalyptol system, azeotropic behavior was indicated, which proved challenging for accurate representation by the models. In contrast, a better agreement between experimental and calculated data was achieved for the other mixtures. None of the systems could be described as ideal mixtures. Overall, the NRTL and UNIQUAC models provided the most reliable correlations.

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Microfluidic systems for separation and preconcentration of ion species using the ion depleted zone

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Microfluidics represents a rapidly developing area of research with applications in modern analytical chemistry and bioengineering. One phenomenon that can be utilized in such systems is ion concentration polarization (ICP), which occurs when an electric potential is applied to a system containing ion-selective membranes. The selective transport of ions across these membranes due to an electric potential difference leads to the formation of two characteristic regions. In one region ions accumulate, forming the so-called ion-enriched zone, while in the other region, referred to as the ion-depleted zone, the ion concentration is significantly lower than in the bulk solution.

In this work we focus on the ICP phenomenon utilized for the separation and preconcentration of various ions based on their charge number. As part of our research, we developed and analyzed a mathematical model of ICP, which requires solving a complex system of partial differential equations, namely the Navier–Stokes, Nernst–Planck, and Poisson equations. Numerical simulations were performed using COMSOL Multiphysics, allowing us to describe the ICP phenomenon in detail and to conduct several parametric studies of the system.

The developed model was subsequently compared with experimental data obtained using a microfluidic device of our own making. These experiments demonstrated that such a device is capable of separating different dyes based on their electrophoretic mobility, thereby giving us another alternative for ion separation in microfluidic devices.

Phytosterol isolation from vegetable oils: Methods and Valorization Potential

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Key words: phytosterols, crude oils, by-products

The European demand for phytosterols (PhS), high-value compounds with hypocholesterolemic, anti-inflammatory and anticarcinogenic properties, is steadily increasing. These compounds are widely used commercially in the pharmaceutical, food, and cosmetic industries.

In Western countries, the average daily intake of PhS from natural sources is 150–440 mg, while vegetarians may consume 1 g/day or more. The European Atherosclerosis Society Consensus Panel specified that a PhS intake of 2 g/day produces a 10 % reduction in low-density lipoprotein (LDL) cholesterol without adverse effects, supporting cardiovascular disease prevention. However, the Western diet is unable to provide an effective dose to achieve a cholesterol-lowering effect. Due to the limited intake of PhS from a typical Western diet and their proven cholesterol-lowering and other health benefits, the isolation of PhS from plant sources is essential to produce fortified foods and supplements that can deliver effective daily doses.

PhS are naturally present in oils from seeds such as sunflower, corn, soybean, olive, and rapeseed. Their concentration and composition depend on the plant source, although refining and processing of the oil can significantly increase their content. Isolation of PhS with high yield and purity from crude oils or refining by-products is a focus of intensive research, with increasing attention on by-products from biofuel production that support circular economy principles.

Our work focuses on the evaluation of vegetable oils through the development of efficient and environmentally friendly processes for the isolation of PhS from oils and refining by-products. Post-fermentation corn oil produced by Envien Group contains about 0.4–2 % PhS in free and esterified forms, making it a promising source for their isolation and efficient valorization of bioethanol by-products. Results suggest that PhS are distributed mainly to side-products from biodiesel production.

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Separation of succinic acid from the mixture of organic acids using pertraction

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Key words: organic acid, pertraction, capillary membrane module, succinic acid, trioctylamine, mathematical model

Organic acids, weak chemical compounds defined by the presence of a carboxyl group, serve as vital components in numerous biochemical and industrial pathways. Among these, succinic acid (a dicarboxylic acid inherently present in plant and animal tissues) has emerged as a vital platform molecule. It finds extensive utilization in the synthesis of pharmaceuticals, cosmetics, food additives, and specialized chemical products. While traditionally synthesized via fossil-fuel pathways, contemporary focus has shifted toward sustainable microbial biosynthesis. Utilizing bacterial strains like *Actinobacillus succinogenes* and *Escherichia coli*, this green alternative leverages renewable feedstocks (including glycerol, agricultural waste streams, and lignocellulosic biomass) to mitigate environmental impacts and curb manufacturing costs. However, bio-based generation introduces downstream challenges, as succinic acid must be isolated from complex fermentation broths containing co-generated byproducts like formic, acetic, and lactic acids. Achieving high-purity yields necessitates advanced downstream processing. To optimize this purification matrix, the integration of multi-stage membrane technologies, specifically microfiltration, pertraction, and membrane crystallization, offers a highly efficient and sophisticated solution for target acid recovery.

In this work the set of equilibrium experiments at different pH with the aqueous solution of mixture of organic acids (succinic, acetic and formic acid) in the equilibrium system water-organic solvent (20 % mass trioctylamine in 1-octanol) were performed and compared with equilibrium experiments for individual organic acids. A strong competition of organic acids for extractant in its mixture was observed which notably decrease its individual partition coefficients in the mixture if compared with the aqueous solution of pure acids. Subsequently, the pertraction experiments (in capillary membrane module) with a model feed phase (aqueous solution of mixture of organic acids in different ratio) were realized at different conditions. The feed solution was kept by either at intrinsic pH with clear water used as stripping phase (both without pH regulation), or with feed phase regulated at pH 5 with strong alkaline stripping phase maintained at pH in range 12-13.5. For better understanding, pertraction experiments were simulated and measured data was predicted using mathematical model of the pertraction process.

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Study of Donnan Dialysis for the Recovery of Valuable Substances from Wastewater

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Key words: Donnan dialysis, anion-exchange membranes, ion-exchange equilibrium, diffusion coefficient estimation, Nernst–Planck equation, wastewater treatment

Nowadays membrane separation technologies are widely applied in various industrial fields, including drinking and wastewater treatment, as well as food and pharmaceutical production. A promising area of membrane technology application is the recovery of valuable substances from wastewater streams, where membrane processes such as electrodialysis and Donnan dialysis can be utilized. One important example is the recovery of lithium from waste streams generated during lithium-ion battery recycling, where membrane processes may provide an effective alternative for the recovery of valuable compounds. Donnan dialysis is a membrane separation process based on the selective transport of ions through an ion-exchange membrane driven by an electrochemical potential gradient. While cation-exchange membranes are commonly used for direct transport of metal ions, anion-exchange membranes can also be applied in recovery processes involving metal salts, where the transport of counter-ions plays an important role in the conversion of the target metal into a recoverable form. A proper understanding of ion transport and ion-exchange equilibria is essential for the design and optimization of such membrane systems. For this purpose, the Nernst–Planck equation is usually used to describe ion transport through ion-exchange membranes. However, this approach represents a relatively complex transport model requiring equilibrium data, such as membrane ion-exchange capacity and selectivity, together with transport properties, such as diffusion coefficients. In practice, simplified approaches based on Fick's law are often used, where the transport process is described by an overall mass transfer coefficient. This work focuses on the experimental study of ion-exchange equilibria and transport properties of investigated anion-exchange membrane in selected binary anion systems involving sulfate, chloride, nitrate, hydroxide, and carbonate ions. Transport parameters, including diffusion coefficients and overall mass transfer coefficients, were determined from experimental data obtained in a CSTR membrane module equipped with an anion-exchange hollow-fiber membrane. The obtained transport parameters were subsequently used in the developed mathematical model for the prediction of ion transport in an independent batch membrane system for selected anion pairs. The comparison of predicted and experimental concentration profiles enabled the evaluation of model accuracy and the applicability of both the Nernst–Planck and Fick approaches for the description of ion transport in Donnan dialysis systems.

Acknowledgments

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Lectures: Reaction engineering and catalysis

Biomass to useful molecules – From batch to continuous operation with the aid of structured catalysts and reactors

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Key words: biomass valorisation, structured reactors, process intensification

The shift from fossil resources to renewable raw materials and sustainable products has been a massive vitamin injection for chemistry and chemical engineering. New catalysts have been discovered, characterized and tested. The trinity for a good heterogeneous catalyst is activity, selectivity and durability. Besides the conventional structures of heterogeneous catalysts, new structures have been developed, such as monoliths, microreactors, solid foams and 3D printed elements. The goal is to combine the benefits of traditional powder catalysts and catalyst pellets, i.e. to minimize the diffusion resistance in the catalyst pores by applying thin catalyst layers but preserving the open structure to minimize the pressure drop. Application of new structures is particularly attractive for chemical applications appearing in the valorization of biomass components to valuable chemicals, food ingredients, pharmaceuticals and fuel components. The shift from batch to continuous production is desirable because continuous operation leads to higher productivity, well-controlled product quality and improved safety. Introduction of structured catalysts and reactors in continuous operation are central elements in process intensification.

Qualitative approach is not sufficient, since the ultimate goal is to gain deep knowledge of the reaction mechanisms and to progress from laboratory to industrial scale. Understanding and modelling thermodynamics, kinetics, transport phenomena and fluid dynamics is the way to breakthrough. The systematic approach is illustrated with several real-life examples, such as hot-water extraction of polysaccharides from forest biomass, hydrolysis of hemicelluloses (arabinogalactan, galactoglucomannan, inulin), as well as hydrogenation and oxidation of monosaccharides (arabinose, galactose, xylose) to sugar alcohols and sugar acids. The power of the new catalyst and reactor technology is discussed, i.e. replacement of slurry and pellet technologies with structured catalysts, such as solid foams and 3D printed structures. Mathematical models for reaction kinetics are obtained from isothermal and non-isothermal batch experiments, after which the feasibility of continuous operation is demonstrated and the parameters for mass transfer and flow pattern are estimated from experiments conducted in continuous mode. Finally, the model elements from batch and continuous operation are merged to working multiphase reactor models, which can be used for predictions in laboratory scale and for process scale-up.

Continuous Xylitol Production on Solid Foam Catalyst: Mass Transport and Kinetic Modelling

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Key words: solid foams, biomass valorization, sugar alcohols, kinetics, mass transfer

The efficient valorization of biomass remains a central challenge in chemical reaction engineering, particularly for three-phase catalytic processes such as hydrogenation. In these systems, a liquid-phase substrate reacts with dissolved gas at the surface of a solid catalyst, coupling hydrodynamics, mass transfer, and intrinsic reaction kinetics. Sugar alcohols such as sorbitol and xylitol, obtained by sugar hydrogenation, are valuable ingredients in alimentary and pharmaceutical products. Conventional slurry reactors using finely dispersed catalysts can reduce internal diffusion limitations, but they complicate catalyst separation and are typically restricted to batch operation. For process intensification, continuous operation is highly desirable. Metallic open-cell foam catalysts represent a promising alternative due to their high void fraction, thin catalytic layers, and excellent heat transfer properties. From a technical viewpoint, continuous operation with solid foams is straightforward, but reactor performance remains strongly governed by liquid distribution, wetting efficiency, dispersion, and gas–liquid and liquid–solid mass transfer, requiring integrated analysis to approach intrinsic kinetic control.

Continuous hydrogenation of xylose to xylitol was investigated using a synthesized Ru/C solid foam catalyst in a parallel screening co-current downflow reactor under varying operating conditions (60–90 °C, 0.25–1.25 mL min^{-1} liquid flow rate, and 0.13–0.39 M xylose concentration). Reactor hydrodynamics were characterized by residence time distribution (RTD) and liquid holdup measurements. The results were interpreted using an axial-dispersion reactor model coupled with a kinetic expression based on non-competitive adsorption of hydrogen and xylose, including external mass transport of the reactants. Temperature and liquid flow rate were identified as key parameters, influencing intrinsic kinetics and residence time, respectively. The analysis quantified gas–liquid and liquid–solid mass transfer contributions. Although solid foams mitigate internal diffusion limitations, external transport resistances remain significant and may limit overall performance. These findings highlight the importance of improving catalyst wetting and interfacial transport to fully exploit foam-based structured catalysts in continuous three-phase hydrogenation.

Co-solvent free conversion of biomass-originated levulinic acid to γ-valerolactone: from molecular level to process design

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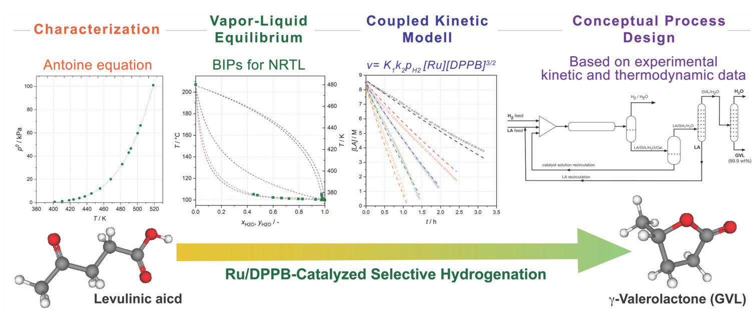
Keywords: hydrogenation, homogeneous catalysis, reaction kinetics

The global efforts to replace fossil-based resources for the chemical industry demand new and innovative strategies for the green production of fuels and platform molecules, among which γ-valerolactone (GVL) stands out as a promising C_5-platform molecule.[1]

We showed that GVL can be readily obtained via catalytic hydrogenation of levulinic acid (LA) in the presence of a catalyst *in situ* generated from $Ru(acac)_3$ and 1,4-bis(diphenylphosphino)butane (DPPB). While numerous investigations have been carried out to develop selective catalyst systems, no experimentally derived kinetic and thermodynamic data-based conceptual process design has been reported for the homogeneous phosphine-modified Ru-catalyzed transformation of LA to GVL. Thus, we aimed to determine the kinetic parameters and demonstrate the continuous production of GVL from LA using our recently published concept of "*from Molecular Level to Process Design (MoLePoD)*".[2]

It was found that the concentration-time profiles of LA followed almost perfect linear trends up to more than 70% conversion, suggesting a formal kinetic order of zero for LA in the rate-determining step. Using a newly developed Coupled Kinetic Model (CKM), it was shown that the rate-determining step is the activation of molecular hydrogen to form the active catalyst for the reduction of LA, leading eventually to the formation of GVL and H_2O. Furthermore, temperature-dependent measurements provided the corresponding activation parameters of $\Delta H^{\ddagger}_{app}$ = 113.5 ± 8.5 kJmol^{-1} and $\Delta S^{\ddagger}_{app}$ = +53.1 ± 20.2 Jmol^{-1}K^{-1}, respectively.[3]



Our contribution will discuss the development of the conceptual process design for GVL production, including vapor-liquid equilibria study, mechanistic study using deuterium isotope labeling, and reaction kinetic measurements.

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Phosphine–free Heck coupling reaction, in 1,4–pentanediol as an alternative biomass–derived medium

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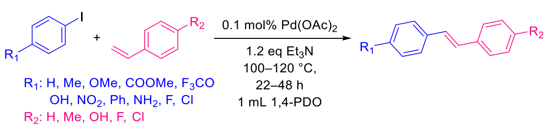
Keywords: Heck reaction, homogeneous catalysis, phosphine–free, green chemistry

In the field of multistep synthesis of biologically active compounds, transition metal–catalyzed cross–coupling reactions have become one of the most powerful tools for the construction of new carbon–carbon bonds. The Pd-catalyzed Heck reaction between an aryl halide and an alkene is a facile protocol to synthesize fine chemicals, including active pharmaceutical intermediates.[1] The reaction is usually carried out in conventional polar aprotic solvents, e.g., DMF or NMP, which are suspected carcinogens.

We have demonstrated that the biomass–originated 1,4–pentanediol (1,4–PDO) could be utilized as an alternative protic polar reaction medium for the homogeneous Ullmann–type C–N coupling reaction of aryl halides and primary or secondary amines.[2] Based on these results, our aim was to broaden the applicability of 1,4–PDO with the Heck reaction.

It was shown that 1,4–PDO can be used as a medium for phosphine–free Pd-catalyzed synthesis of several stilbene derivatives. Cooling the reaction mixture to room temperature resulted in the product precipitating as brownish crystals, facilitating product isolation.

In our presentation, we will discuss the effects of various reaction parameters (e.g., temperature, catalyst precursor, base, and para–substituent derivatives of the substrates) on system activity (Scheme 1), the general low E–factor isolation method, and the parallel solvent–catalyst recycling.[3]



Scheme 1 *Pd-catalyzed Heck-coupling of iodobenzene and its para-substituted derivatives with styrene and its para-substituted derivatives*

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Lectures: Material engineering and design

Crystal Engineering of Low-Dimensional Metal Halide Hybrids for In-Memory Computing Technologies

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Key words: bismuth iodide hybrids, resistive switching devices, neuromorphic computing

Low-dimensional metal halide hybrids have recently emerged as promising materials for adaptive electronic and neuromorphic devices due to their structural versatility and defect-mediated transport properties. In this research journey, a crystal engineering approach was employed to systematically control the dimensionality and electronic structure of halide complexes through modification of the organic component. Pyridinium-based cations were shown to direct the assembly of metal–halide units from isolated 0D clusters to extended 1D chains through hydrogen bonding and electrostatic interactions, enabling cation-dependent band-gap modulation and influencing resistive switching behaviour in metal–insulator–metal devices [1-4]. Low-dimensional systems exhibited enhanced resistive switching characteristics associated with defect-assisted charge transport. The design strategy was further extended to aliphatic cations and organic dications, introducing additional structural stabilization and tunable connectivity within the inorganic framework. These results highlight the potential of structurally engineered metal halide hybrids as a versatile platform for low-power neuromorphic and in-memory computing technologies, encompassing both lead-free and transition-metal-based systems [1-4].

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Electronic Structure and Reactivity Descriptors of BN-Doped Naphthalimide–Carbazole Bipolar OLED Emitters: A DFT/TD-DFT Study

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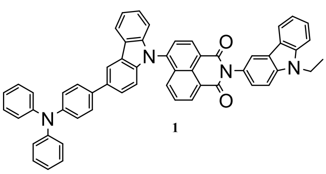
Abstract

Organic light-emitting diode (OLED) technologies depend on precise control of molecular electronic structure to enable efficient charge transport and stable emission. In this context, naphthalimide–carbazole-based bipolar emitters offer a versatile donor–acceptor framework for tuning optoelectronic properties. The molecular structures studied include three reference compounds (1–3), where carbazole and triphenylamine units act as electron-donating segments, and the naphthalimide core functions as the electron-accepting unit. A boron–nitrogen (BN) isosteric doping strategy is applied to these structures to systematically explore changes in electronic properties. BN units are selectively incorporated into the acceptor core and nearby aromatic regions, adjusting the distribution of frontier molecular orbitals while maintaining the overall π-conjugated framework of the parent molecules. Density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations are used to assess key electronic features, including HOMO–LUMO energy levels, global reactivity descriptors, and molecular electrostatic potential (MEP) maps. The findings show that structural differences among compounds 1–3, especially in donor strength and substitution patterns, significantly impact orbital localization and charge distribution. Comparing these results reveals that BN substitution further enhances electronic polarization and influences donor–acceptor interactions based on the substitution site. These outcomes highlight that both the molecular architecture and BN-doping strategy are crucial in shaping electronic behavior. Overall, this study offers a structure-based computational perspective on BN-doped naphthalimide–carbazole systems and provides guiding principles for designing efficient bipolar OLED emitter materials.



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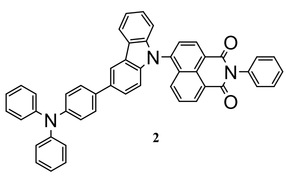

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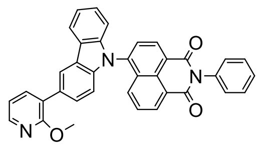

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Key words: OLED, BN-doping, bipolar emitters, TADF, DFT

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Integration of microstructured surfaces with microfluidics for dynamic biofilm research

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Key words: biofilm, microstructured surfaces, microfluidics

Bacterial biofilms are structured microbial communities embedded in a self-produced extracellular matrix that enhances their resistance to environmental stresses and antimicrobial agents. Understanding how surface topography interacts with hydrodynamic conditions to regulate biofilm formation remains a key challenge in biofilm research. This work presents a microfluidic platform that integrates microstructured polydimethylsiloxane (PDMS) surfaces and enables controlled investigation of *Escherichia coli* behavior under defined flow, shear stress, and nutrient transport, bringing the system closer to physiologically relevant environments compared to conventional static models. The experimental workflow consists of static and dynamic experiments supported by microscopy to quantify early attachment, microcolony formation, and biofilm morphology, while assessing how microstructure-induced local hydrodynamics shape adhesion and spatial organization. The results establish relationships between surface geometry, shear conditions, and resulting biofilm architecture, providing a basis for the rational design of surfaces that either suppress biofilm formation or enable controlled biofilm growth in applications such as medical devices and biofilm-based functional interfaces.

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Processing-Driven Porosity Engineering in Resorcinol–Formaldehyde-Derived Carbon Gels for High-Performance Supercapacitors

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Key words: carbon gels; resorcinol–formaldehyde; sol-gel polycondensation; hierarchical porosity; drying; activation; supercapacitor

Resorcinol–formaldehyde (RF)–derived carbon gels are widely recognized as promising electrode materials for electrochemical double-layer capacitors (EDLCs) due to their tunable pore structure, high carbon yield, and good mechanical, thermal, and electrical properties. This work examines how sol–gel chemistry, drying-induced capillary stresses, carbonization temperature, and activation methods collectively influence the development of hierarchical porosity, with particular focus on optimizing the micro–mesopore balance for improved charge storage.

The pore structure is largely established during the sol–gel polycondensation stage. Key synthesis parameters, including the resorcinol-to-catalyst ratio, initial pH, and solids content, control the formation of interconnected polymer networks. Adjusting these variables allows systematic tuning of particle size, pore size distribution, and network connectivity in the resulting carbon materials. Drying plays a critical role in preserving this structure. Capillary stresses generated during ambient or vacuum drying can lead to partial pore collapse and reduced accessibility. In contrast, solvent exchange and freeze-drying help alleviate these stresses, resulting in better retention of mesoporosity and improved internal surface accessibility. Consequently, the drying pathway strongly affects both pore connectivity and the efficiency of subsequent activation. Carbonization further modifies the pore structure and material properties. Higher temperatures generally enhance microporosity, electrical conductivity, and structural ordering, but may also reduce surface oxygen functionalities, affecting wettability and electrode–electrolyte interactions. The overall electrochemical performance therefore depends on a balance between conductivity, surface chemistry, and pore architecture. Additional tuning of microporosity is achieved through physical (CO_2) and chemical (KOH) activation. The effectiveness of these treatments is closely linked to the initial mesoporous framework established during drying, which governs ion transport and double-layer formation.

Overall, this study highlights how coordinated control over synthesis and post-treatment steps enables the design of RF-derived carbon gels with tailored porosity for high-performance supercapacitor applications.

Lectures: Pharmaceutical engineering and processes

Characterization and identification of anthocyanins in natural extracts

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Key words: anthocyanins, natural substances, analytical methods, bioactive compounds

Over the years, considerable interest has developed in fruits and vegetables containing high concentrations of flavonoids, due to their potential biological effects and health benefits. They are among the powerful antioxidants that protect cells from oxidative stress, reduce inflammation, and support cardiovascular health. They are responsible for the characteristic coloration of many plant sources such as blueberries, chokeberries, grapes, etc. In nature, six basic anthocyanidins are most commonly found, which differ in the number and position of -OH and -OCH_3 groups on the aromatic ring, which affects their color, stability, and antioxidant properties. In addition to the basic aglycones, natural substances also contain their glycosides, to which a sugar is attached, e.g. glucose, galactose, arabinose.
The aim of the work is to identify anthocyanins present in several selected natural extracts. Before measuring the sample using the selected analytical method, material preparation and separation of bioactive compounds using lyophilization, extraction, and ultrasonic homogenizer are necessary. The obtained results allowed the identification of several anthocyanidins and their glycosides and provided a more detailed view of their representation in the analyzed extracts.

Study of 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 one of the main limitations of the freeze-drying process, as it introduces unpredictability and variability between samples and within the same batch. The randomness is because ice nucleation – the moment when crystals start to form in a solution – does not always occur at the same temperature or at the same time. The result is differences in the size, shape, and distribution of ice crystals, which in turn determine the microscopic structure of the final product. Samples that start to nucleate earlier (at a higher temperature) tend to form larger ice crystals, resulting in larger pores and lower cake resistance. Conversely, later nucleation leads to smaller crystals and a more compact structure, which slows down sublimation. Variability in nucleation is therefore a critical problem, especially in industries where high reproducibility and quality are required, such as the pharmaceutical, biotechnology, or food industries. However, the underlying mechanism of random nucleation behavior is not yet fully understood, as it depends on several interrelated parameters, such as sample volume, solution composition, and vial placement in the lyophilizer. The results of this study showed that all of these factors contribute to the observed heterogeneity in nucleation.

Lectures: Energetická transformácia priemyslu & Zhodnocovanie vedľajších prúdov z výroby (SK industry session)

Posters

Posters: Energy transition and circular economy

Performance Analysis of Single to Triple-Stage Evaporation–Crystallization Systems for Efficient Brine Processing

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Abstract
Evaporation and crystallization are the most energy-intensive operations in brine processing, and their optimal design is of great importance to the brine processing industry. In this study, single-stage and triple-stage evaporation systems with crystallization were designed, and their energy and economic efficiency were compared and analyzed. In addition, two operation configurations were studied: without a steam ejector and with a steam ejector. Membrane distillation was considered as an alternative solvent removal technology. The models were built in Aspen Plus simulation software. Specific steam consumption, total energy consumption, capital costs, and operating costs were taken as the evaluation indicators. The results showed that the thermal efficiency of evaporation was improved significantly with the increase of evaporation stages, and the three-stage system had the lowest specific energy consumption. However, the capital investment and complexity of the system increased with the increase in evaporation stages. The integration of steam ejectors further reduced steam consumption by partial vapor recompression. The energy-saving effect was obvious in all configurations. The results showed that the relative advantage of the steam ejectors was more obvious in the three-stage system. The economic evaluation results showed that there was a compromise between capital costs and operating costs. The single-stage system had the lowest investment cost, while the three-stage system had the lowest total cost in the long run, especially with the ejectors. The energy cost, feed concentration, and plant capacity had significant effects on the optimal design of the system in all considered cases. The research results provide practical references for the design and selection of evaporation–crystallization systems, with further research to be dedicated to a generalized framework for evaluation and optimization of the brine processing technologies.

This study was supported by the Slovak Research and Development Agency under contract no. VV-MVP-24-0365.

Posters: Bioprocess and biotechnology

Analysis of the Efficiency of Acid Thermohydrolysis of Lignocellulosic Biomass (Willow Chips) Using Conventional and Microwave Heating in the Biogas Production Process

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Key words: acid thermohydrolysis, lignocellulosic biomass, anaerobic digestion, methane yield, microwave heating

Biogas is considered one of the most stable renewable energy sources; however, the efficient utilization of lignocellulosic biomass remains limited due to its complex structure and low biodegradability. Willow chips, characterized by high lignin content, represent a promising but recalcitrant substrate requiring effective pretreatment to enhance methane production.

The aim of this study was to evaluate the effect of acid thermohydrolysis on the efficiency of biogas production from willow biomass and to compare two heating methods: conventional and microwave-assisted heating. Pretreatment was carried out using hydrochloric acid (HCl) at temperatures of 110°C, 120°C, and 130°C, with a residence time of 20 minutes.

The application of acid thermohydrolysis significantly increased the solubilization of organic compounds. Chemical oxygen demand (COD) increased from 10.2 g/L in the control sample to 14.7 g/L for the microwave-assisted variant at 120°C, indicating enhanced availability of biodegradable matter. A substantial increase in soluble sugars was also observed, with glucose rising from 14 mg/L to 124 mg/L and xylose from 194 mg/L to 412 mg/L, confirming effective hemicellulose hydrolysis.

At the same time, the formation of inhibitory compounds was detected. The concentration of hydroxymethylfurfural (HMF) increased with temperature, reaching 24.78 mg/L for conventional heating at 130°C, indicating thermal degradation of sugars. In contrast, the concentration of phenolic compounds decreased with increasing temperature, suggesting partial lignin breakdown.

Biogas production was significantly improved after pretreatment. The highest yield was obtained for microwave-assisted thermohydrolysis at 120°C (800.0 Nml/g VS), corresponding to an increase of approximately 45% compared to the control (550.6 Nml/g VS). Conventional heating also enhanced performance, with the highest yield of 773.2 Nml/g VS at 120°C. At 130°C, a

decrease in biogas production was observed, likely due to the formation of inhibitory by-products.
The methane content in biogas remained relatively stable across all experimental variants, ranging from 59.8% to 60.6% CH_4, indicating that pretreatment mainly affected the quantity rather than the quality of biogas.
In conclusion, acid thermohydrolysis is an effective method for improving the biodegradability of lignocellulosic biomass. Microwave-assisted heating enhances process efficiency compared to conventional methods; however, excessive process severity leads to inhibitor formation. The optimal conditions were identified at 120°C, where the most favorable balance between substrate solubilization and inhibitor generation was achieved.

The research was funded as part of the project "Development of pretreatment technologies for lignocellulosic substrates prior to conversion into second-generation biofuels" under the LIDER XIII programme, funded by the National Centre for Research and Development, grant no. LIDER 13/0050/2022. Amount of funding: PLN 1,410,000.00

Continuous cultivation of Chlorella vulgaris using condensate derived from agricultural biogas digestate

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Key words: *Chlorella vulgaris*, digestate, condensate, ammonium, microalgaeds,

The search for alternatives to conventional synthetic culture media, capable of ensuring both high biomass productivity and sufficient availability of essential macronutrients such as nitrogen, remains a key factor determining the feasibility of large-scale microalgae cultivation. In this context, the present study explores the use of digestate as a nutrient source for microalgal growth. Digestate, obtained as a by-product of anaerobic methane fermentation in an agricultural biogas plant, was subjected to thermo-pressure fractionation. This process enabled the separation and recovery of a liquid fraction rich in nitrogen compounds, which was subsequently applied as a culture medium.

The experimental work focused on the cultivation of *Ch. vulgaris*, a widely studied green microalga with high biotechnological potential.

Biomass production was carried out in tubular photobioreactors with a working volume of 70 L, using a culture medium prepared based on the chemical composition of 3N-BBM+V. Nitrogen compounds in the culture medium were derived from condensate obtained during the thermal treatment of digestate originating from an agricultural biogas plant. A 0.25% dose of nitrogen compounds from the standard culture medium was added to the reactors and supplemented, in varying proportions, with ammonium compounds contained in the condensate.

Microalgae were cultivated under semi-continuous conditions. Following biomass growth, ammonium compounds were automatically dosed using pumps to maintain the desired concentration level. Three nitrogen loading variants were tested: 50, 100, and 150 mg N/L.

The results confirm that digestate-derived condensate can serve as an efficient nutrient source for microalgae cultivation while enabling simultaneous nutrient recovery and biomass production.

Optimal nitrogen concentration was identified at ~100 mg N/L. The system exhibited characteristics typical of continuous cultivation, with an initial growth phase followed by the establishment of steady-state conditions. The maximum biomass concentration (1.8 g/L) was achieved at a nitrogen loading of 100 mg N/L. At lower nitrogen loading, nutrient limitation was observed, resulting in reduced biomass accumulation (~1.1 g/L). In contrast, higher nitrogen loading led to signs of inhibition and decreased productivity. Biomass production and nutrient removal can be effectively coupled in a continuous system. A dynamic equilibrium was established after approximately 6–8 days, as indicated by stable biomass concentrations.

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Controlling Trajectories of Iron oxide Nanoparticles by Free-flow Electrophoresis for Bioapplications

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Key words: SPIONs, continuous separation, enantiomers, free-flow electrophoresis

Superparamagnetic iron oxide nanoparticles (SPIONs) possess distinctive magnetic properties that arise from their nanoscale dimensions and superparamagnetic behavior. These characteristics make them exceptionally suitable for a broad spectrum of biomedical applications. However, the full potential of SPIONs relies on the ability to precisely manipulate their movement and separation in continuous flow systems. This study explores the use of Free-flow Electrophoresis (FFE) as a versatile tool for controlling the trajectories of functionalized SPIONs based on their electrophoretic mobility.
The cornerstone of this study is a predictive model designed to precisely control and predict the trajectories of functionalized SPIONs within a Free-flow Electrophoresis (FFE) system. This framework is applied to optimize two high-precision bio-applications: enantioseparation and cancer cell diagnostics. In enantioseparation, chiral selectors on the SPION surface enable the separation of enantiomers based on their differing electrophoretic mobilities. In diagnostics, antibody-conjugated SPIONs target malignant cells, such as the HT-29 line, for continuous isolation. Critically, the FFE system serves as an essential clean-up stage by removing unbound nanoparticles that would otherwise cause signal interference, ensuring high-purity separation and more accurate downstream analysis. This synergy between trajectory modeling and FFE purification provides a robust platform for advanced diagnostic and preparative biomedical tasks.

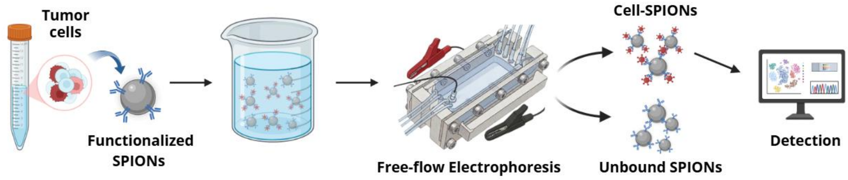

Figure 1: Schematic workflow of the FFE-mediated diagnostic platform.

Dual Catalytic Functions of Human Carbonic Anhydrase II in the Tandem Synthesis of Chiral Halohydrins and Epoxides from α-Haloketones

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Key words: human carbonic anhydrase II; α-haloketones; halohydrins; epoxides; biocatalysis; stereoselective reduction, mutant

Human carbonic anhydrase II (hCA II) is a zinc-dependent metalloenzyme best known for catalyzing the reversible hydration of carbon dioxide. Beyond its physiological role, hCA II can display catalytic promiscuity in hydride-transfer reactions from silanes to carbonyl compounds, providing a useful platform for stereoselective biotransformations under mild conditions. In this work, we report a single-enzyme cascade approach for the conversion of α-haloketones into chiral halohydrins and the corresponding epoxides using hCA II and phenylsilane as reducing agent.

The transformation proceeds through the enzyme-mediated reduction of the carbonyl group, affording enantioenriched halohydrins as key intermediates. These compounds are valuable bifunctional building blocks, as they contain both a stereodefined alcohol center and a reactive carbon-halogen bond. Moreover, they can undergo intramolecular dehydrohalogenation to generate epoxides, transferring the stereochemical information established during the reduction step to strained three-membered heterocycles with high synthetic utility.

The method was investigated using purified hCA II and whole-cell biocatalysts, as well as mutant variants generated to modulate catalytic performance and stereoselectivity. α-Haloacetophenone derivatives afforded predominantly *R*-configured halohydrins and the corresponding phenyl oxiranes, while chloropropiophenone substrates showed substrate-dependent stereochemical outcomes. The hCA II-mediated reduction of 2-chloropropiophenone preferentially afforded *R*-configured halohydrins, whereas 1-chloropropiophenone favored *S*-configured alcohol products. In both cases, the corresponding epoxides were generated through intramolecular ring closure of these stereodefined halohydrin intermediates.

The configuration of the newly formed alcohol center, together with that of the adjacent halogen-bearing carbon, defines the diastereomeric distribution of the intermediates and governs the stereochemical course of subsequent ring closure. Notably, for para-substituted derivatives bearing 4-Br, 4-Cl, and 4-F groups, the V121A mutant induced an inversion of epoxide configuration, affording the *S*-epoxide while the halohydrin intermediate retained the *R* configuration. These results highlight the potential of hCA II as an engineered biocatalyst for stereodivergent access to chiral halohydrins and epoxides from readily available α-haloketones.

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Enriching drinking yogurt with galactooligosaccharides

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Key words: prebiotics, galactooligosaccharides (GOS), β-galactosidase, yogurt, syneresis, antioxidant activity

Food fortification is one of the most important processes for improving the quality and increasing the nutrient value of food. In this context, there is growing interest in functional ingredients, including those related to gastrointestinal function, and in particular prebiotics.
The aim of this study was to produce yogurts enriched with galactooligosaccharides (GOS) and the *in situ* synthesis of GOS in yogurt on quality of drinking yogurt. The yogurts were prepared supplemented with 3, 4, 5, and 6%, GOS as well as yogurts with added NURICA preparation in various amounts. The yogurts were analyzed after fermentation and after 21 days of storage at 4°C. During the study, the acidification kinetics of the yogurt, its chemical composition, the profile of carbohydrates, volatile components, and microbiological composition. The syneresis and water-binding capacity of the yogurt, its antioxidant activity, color, microstructure, and organoleptic characteristics were also evaluated. The results of the study showed that the addition of the GOS concentrate and the β-galactosidase does not interfere with the fermentation process or the microstructure of the yogurts, ensuring high antioxidant activity. Although the fortified products had changed color and exhibit greater syneresis after 21 days of storage, their basic microbiological parameters and the quality parameters of the yogurt remained appropriate and typical of drinkable yogurt.

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Extruded beetroot preparation as an enriching ingredient in gluten-free bread

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Key words: beetroot, fiber, gluten-free bread

Bread is one of the fundamental components of the human diet. In its traditional form, it is based on gluten-containing cereals, mainly wheat and rye. In recent years, however, a rapid increase in demand for gluten-free products has been observed. On the one hand, this results from growing prevention efforts and awareness of gluten-related disorders (including celiac disease and wheat allergy), for which the implementation of a strict elimination diet is the only effective form of therapy. On the other hand, voluntary gluten avoidance is becoming increasingly popular, motivated by the perception of such a diet as more beneficial for overall health. However, gluten-free bread is characterized by a lower nutritional value. Another challenge is achieving an appropriate bread structure in the absence of gluten, which is responsible for structure formation.
The aim of this study was to develop a formulation and evaluate the effect of adding a dietary fiber preparation from red beetroot on the physicochemical, textural, and sensory properties of gluten-free bread.
The research material consisted of gluten-free breads based on corn and potato starches. In the basic formulation, the starches were partially replaced with a fiber preparation at levels of 5%, 7.5%, and 10%. The effect of the addition on loaf volume, dry matter content, water activity, color, texture, and sensory characteristics was evaluated.
It was found that the addition of beetroot fiber at a level of 7.5% allowed for the production of gluten-free bread of high quality and consumer acceptance. Higher concentrations (10%), despite improving loaf volume, negatively affected crumb texture, making it excessively hard and gummy.

From insect protein to functional ingredients: Spray-dried microencapsulation of bioactive peptides from *Tenebrio molitor*

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Key words: *Tenebrio molitor*; Enzymatic hydrolysis; Microencapsulation; Bioactive peptides

Insects are recognized as promising alternative sources of protein, due to their ability to convert low-value organic substrates into nutrient-rich larval biomass with high feed conversion efficiency and low environmental impact. Among them, mealworm larvae (*T. molitor*, TM) represent a scalable and sustainable resource. However, current industrial applications still rely on whole-larvae meals, where chitin-protein interactions may limit protein bioavailability, and despite rapid growth of the edible insect sector, products based on purified bioactive peptides remain scarce. Converting mealworm proteins into encapsulated antioxidant peptide ingredients represents a shift from commodity insect proteins toward high-value precision nutrition products.

This study explored the potential of *T. molitor* protein isolate as a sustainable source of bioactive peptides and addressed the challenges related to bioavailability and instability. Enzymatic hydrolysis with alcalase efficiently generated peptide-rich hydrolysates with favourable amino acid composition and significantly enhanced antioxidant capacity, including improved scavenging of multiple free-radical species. Nevertheless, their application remains challenged by bitterness, hygroscopicity and sensitivity to environmental factors.

Therefore, the obtained hydrolysates were further stabilised by spray drying microencapsulation using maltodextrin as a carrier. The effect of formulation parameters, including the hydrolysate:carrier ratio, was evaluated through process yield, encapsulation efficiency and loading capacity, with optimal conditions at a 1:6 ratio and 25% dry matter. Scanning electron microscopy (SEM) revealed predominantly spherical microparticles (2 to 20 µm), while FTIR analysis confirmed successful incorporation within the maltodextrin matrix.

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Highly Enantioselective Continuous Flow Henry Reactions Enabled by Immobilised Hydroxynitrile Lyases

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Keywords: flow chemistry, Henry reaction, heterogeneous biocatalysts, hydroxynitrile lyases, monolithic structural microreactors

Exploiting the catalytic promiscuity of hydroxynitrile lyases (HNL), we applied these enzymes in asymmetric Henry reactions under continuous flow conditions. Biocatalytic C–C bond formation remains challenging due to limited enzyme stability and incompatibility with non-conventional reaction media. Here, we present an efficient strategy combining enzyme immobilisation with continuous flow processing to enable highly enantioselective Henry reactions.

The enzymes were immobilised on organically modified silica monolithic microreactors and applied in a biphasic system under continuous flow conditions. This setup enabled efficient synthesis of chiral β-nitroalcohols, important building blocks in the synthesis of biologically active compounds, from aromatic aldehydes and nitroalkanes.

The system delivered (*R*)-1-phenyl-2-nitroethanol with excellent enantioselectivity (>99% ee) and demonstrated stable performance during extended operation. The monolithic reactor architecture ensured efficient mass transfer and robust catalyst integration, while spectroscopic analysis confirmed stable enzyme immobilisation, highlighting the advantages of covalent attachment.

Overall, this work establishes a robust and scalable platform for asymmetric Henry reactions, thereby expanding the applicability of HNL in continuous-flow biocatalysis.

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In Search of Suitable Amine Dehydrogenase: Identification and Development of AmDHs with Industrially Relevant Substrate Scope

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Key words: amine dehydrogenase, biocatalysis, chiral amines, homology, molecular dynamics, phylogeny, flavor and fragrance

Abstract:
Amine dehydrogenases (AmDHs) are NAD(P)H-dependent oxidoreductases catalyzing the reductive amination of carbonyl compounds into amines. Due to their excellent stereoselectivity, simplified reaction stoichiometry, and environmentally favorable reaction conditions, AmDHs represent attractive biocatalysts for pharmaceutical, fine chemical, and flavor and fragrance industries. However, only a limited number of naturally occurring AmDHs active toward short-chain aliphatic and hydroxy-functionalized substrates have been described.
The aim of this work is to identify and characterize novel AmDH candidates with substrate specificity relevant for industrial applications. A substrate panel consisting of 15 structurally diverse aldehydes, ketones, hydroxyaldehydes, and hydroxyketones was designed to guide enzyme selection and evaluation. A comprehensive literature survey covering 120 scientific publications resulted in a curated database containing information on 218 AmDH enzymes and variants, including substrate scope, catalytic activity, cofactor preference, and reaction conditions.
Based on their diverse substrate specificity, 53 enzymes were selected for phylogenetic analysis using the iTOL platform. Ten representative enzymes with distinct phylogenetic distribution and substrate preference were further analyzed by homology searches against publicly available genomic databases. Structural analysis involving molecular docking, molecular dynamics simulations, and SmarTSzyme analysis was subsequently performed for selected candidates to identify structural determinants affecting substrate specificity and to propose potentially beneficial mutations.
The combined bioinformatic workflow enabled the identification of several promising AmDH candidates suitable for heterologous expression and experimental validation. The presented approach provides an effective strategy for the discovery and engineering of novel AmDHs with potential applications in sustainable synthesis of chiral amines and amino alcohols.

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Ionic liquid-tuned formate dehydrogenase-carbonic anhydrase enzyme cascades: temperature- and structure-dependent activity enhancement

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Key words: Formate dehydrogenase; imidazolium-based ionic liquids; enzyme cascade; carbonic anhydrase; temperature-dependent enzyme activity

The activity of formate dehydrogenase (FDH) was investigated in imidazolium-based ionic liquid (IL) – phosphate buffer systems across a wide range of solvent compositions (IL/buffer ration= 0-60 V/V %) and temperatures (T= 37 – 50°C), both as a standalone enzyme and in an FDH – CA (carbonic anhydrase) enzyme cascade. The highest FDH activity was achieved in the presence of $BmimMeSO_3$ (20m/v%; 50°C), where the maximum specific activity reached 9.05 µmol min^{-1}, corresponding to a 31.21-fold increase compared to the aqueous reference system (0% IL, 50°C). In the FDH-CA cascade system, the incorporation of CA led to a further enchantment of catalytic performance, yielding an activity increase of 1.124-fold (12.4%) compared to FDH alone.
Statistical analysis revealed that the IL concentration, temperature and the structural properties of both the cation and anion significantly influence enzyme activity, with pronounced interaction effects between these parameters. Based on multivariate statistical evaluation, an optimal parameter window was identified that maximizes FDH activity and cascade efficiency. These results demonstrate that properly tuned IL-buffer systems enable enhanced high-temperature operation and efficient integration of FDH-CA enzyme cascades, providing a promising platform for advanced bio- and bioelectrochemical C1 conversion processes.
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Optimization of the enzymatic synthesis of galactooligosaccharides

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Key words: galactooligosaccharides (GOS), β-galactosidase

Galactooligosaccharides (GOS) are prebiotic oligosaccharides that have a beneficial effect on human health by modulating the intestinal microflora. Their prebiotic properties are widely used in the prevention of gastrointestinal diseases, as well as in improving metabolic and immune health. Due to these properties, GOS are used in the food industry, especially in functional foods.
The aim of this study was to analyze the effectiveness of the GOS synthesis using NURICA preparation. The reactions were carried out at 20 °C, 40 °C, and 60 °C, and the process was optimized using the statistical analysis, taking into account selected key parameters for the course of reaction. The reaction kinetics were analyzed using liquid chromatography with a refractometric detector (HPLC-RID) and a evaporative light scattering detector (HPLC-ELSD). The optimal conditions for GOS synthesis in the NURICA-catalyzed reaction are: 40 °C, a lactose concentration of 40%, and a reaction time of 3 hours. As a result of this process, a GOS synthesis yield of 32.28% and a lactose hydrolysis degree of 54.33% were achieved.

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.

Overcoming Mass Transfer Limitations in hCAII-Catalyzed Bioreduction of Bulky Ketones via Pulsed Phenylsilane Addition

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Key words: human carbonic anhydrase, stereoselective reduction, mass transfer limitations, pulsed addition, metal free catalysis

Human carbonic anhydrase II (hCAII) facilitates the abiotic, enantioselective reduction of ketones into chiral alcohols, utilizing phenylsilane as a hydride donor. While the conventional protocol—employing three equivalents of phenylsilane in a 30% (v/v%) DMSO:water mixture—yields excellent performance for soluble model substrates, it is largely ineffective for the bulky, poorly water-soluble ketones typically required for fine chemical synthesis. We have identified a fundamental kinetic bottleneck: the slow mass transfer of hydrophobic substrates into the hCAII active site occurs at a rate that cannot compete with the inherent instability of phenylsilane, which is prone to degradation and volatilization. At low concentrations, this kinetic mismatch is intensified, resulting in poor conversions even when excess reagents are provided.

Our methodology—utilizing pulsed phenylsilane addition—addresses this by maintaining a consistently high concentration of the hydride donor throughout the prolonged substrate ingress phase. When applied within NMP:water or DMSO:water solvent systems, this strategy yielded significantly higher conversions for 2-acetylnaphthalene compared to traditional single-dose methods. Observations using 4-chloroacetophenone as a model substrate provided a critical breakthrough: the success of the reaction is governed by the absolute concentration of phenylsilane rather than the stoichiometric ratio. Low concentrations proved unsuccessful regardless of excess equivalents, whereas high, sustained concentrations achieved success using only two total equivalents.

Detailed extraction analysis further revealed that the precipitation of substrates and products during the workup phase often skews apparent conversion data, reinforcing the conclusion that mass transfer is the primary rate-limiting factor. By decoupling substrate solvation from hydride availability, pulsed delivery allows for industrially viable concentrations (>10 mM) even with challenging, poorly soluble ketones. Chiral chromatography confirms that these gains in efficiency do not compromise high enantioselectivity. Ultimately, this concentration-driven approach bypasses the constraints of fixed-equivalent protocols, establishing hCAII as a robust and practical biocatalyst for the synthesis of chiral alcohols from demanding substrates.

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Structured Hydrogel Reactors for Continuous Enzymatic Production of Allicin

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Key words: FRESH bioprinting, allicin, enzyme immobilization, packed flow reactor

Allicin, a broad-spectrum antimicrobial compound derived from garlic, is produced by enzymatic conversion of alliin catalyzed by alliinase. Despite its promising biological activity, this system is limited by allicin's high reactivity, which can lead to gradual enzyme inactivation via thiol modification, interaction with Pyridoxal-5′-phosphate (PLP) cofactor, and physical hindrance of the active site, reducing the efficiency of conventional batch processes.

This work investigates the continuous production of allicin in a plug-flow reactor using immobilized alliinase entrapped in 3D-printed hydrogel structures, which provide a high surface-to-volume ratio. Freeform Reversible Embedding of Suspended Hydrogels (FRESH) bioprinting is employed to fabricate constructs with defined internal architecture. Different geometries, including gyroid and hexagonal infill, are used to study the effect of structure on transport and catalytic performance.

Compared to conventional immobilization approaches such as randomly packed hydrogel beads, structured architectures offer improved control over flow distribution and mass transport. Interconnected channel networks reduce diffusion distances, minimize stagnant zones, and provide more uniform exposure of the enzyme to the flowing substrate. At the same time, the absence of random packing should lead to lower pressure drop and more predictable hydrodynamic behavior.

The printed hydrogel modules are assembled into a modular packed-bed configuration and operated under continuous flow. The system is evaluated for substrate conversion, enzyme stability, and operational cycles, with direct comparison to batch conditions. Particular attention is given to the extent of enzyme immobilization and its physical retention within the hydrogel matrix during operation.

The combination of continuous flow and controlled internal architecture is expected to mitigate enzyme deactivation by limiting local accumulation of reactive products and by-products, reducing oxidative stress and pH shifts, and improving transport conditions. This approach provides a platform for studying the relationship between reactor design and biocatalytic performance and may contribute to more efficient utilization of reactive enzymatic systems by reducing enzyme consumption, improving recovery, and increasing product yield.

Synthesis of hydroxypatite-based bioceramics using a mechanochemical-thermal approach and biocompatibility testing

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Key words: animal model, bioceramics, embryotoxicity, hydroxyapatite

The aim of our work was to prepare a hydroxyapatite (HA)-based bioceramic material in powder form via mechano-chemical synthesis, using eggshells as a source of calcium. The products were characterized using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and thermal analysis (TG/DTA). The biocompatibility of the synthesized samples was subsequently tested *in vivo* using a chicken embryo (*Gallus gallus domesticus*) model, during which we observed morphological and developmental responses to the presence of the material. We used the CHEST II methodology to assess embryotoxicity and teratogenic potential. We used 32 fertilized hatching eggs, divided into 4 groups. The first group was the control group, without the application of HA or saline (n = 9); the second group was the control group, with the application of 100 µl of saline (n = 6). The third group was the experimental group, with the application of 50 mg of HA (n = 9). The fourth group received 50 mg of hydroxyapatite in the form of a suspension in 100 µl of saline solution (n=8). The combined group allowed us to observe differences in the bioavailability and diffusion behavior of HA when applied in dry form and in suspension form. The test substance was applied to the surface of the embryo, to the intact inner sub-shell layer (*membrana papyracea*), while maintaining the integrity of extraembryonic structures. We used the CHEST II methodology to assess embryotoxicity and teratogenic potential. In the evaluation we monitored parameters such as embryo weight, heart weight, and liver weight, which varied depending on the substance administered. It was found that no significant differences were observed between the individual groups in either total embryo weight or heart weight. However, liver weight increased significantly following the administration of hydroxyapatite in saline, indicating better diffusion and bioavailability of HA in suspension form. We also concluded that the prepared biomaterial in powder form exhibits neither embryotoxicity nor teratogenicity.

This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-23-0372 and VEGA 1/0373/24.

The influence of particle size on oil extraction yield: Kinetic study and assessment of physicochemical properties of cherry pit oil for biodiesel production

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Key words: Fruit waste; Sour cherry pit oil; Solvent extraction; Biodiesel; Extraction kinetics

Alternative feedstocks and agro-industrial by-products are low-cost resources for sustainable biodiesel production. Fruit processing generates millions of tons of by-products suitable for energy recovery. Fruit kernels are recognised as exceptional sources of high-quality oil; however, utilisation of the whole fruit pit and simplification of the extraction process can further improve biomass valorisation. The pits remaining after sour cherry processing (Oblačinska variety, *Prunus cerasus* L.), with an oil content of approximately 22% (wb), were used as a substrate for oil recovery using solvent extraction (hexane; S/L 1:10; 65 °C) and the Soxhlet method. Oil yield was examined using three particle size fractions: d < 450 µm, d < 900 µm and d > 900 µm. The obtained oils were analysed for fatty acid composition and key physicochemical properties.
The kinetics of oil extraction was studied under optimal conditions and the best mathematical model was selected to fit the data. The results showed that cherry pit particle size significantly affected oil yield. The highest yield was obtained with the fraction d < 450 µm using both, solvent and Soxhlet extraction. Particle sizes above 450 µm significantly reduced oil yield. The oil extraction kinetics was described by a first-order kinetic model, showing good agreement between predicted and experimental values, revealing that diffusion was the main limiting factor in the oil extraction. The obtained oils showed a high degree of unsaturated fatty acids, with oleic and linoleic acids being the dominant ones. Acid number, saponification and peroxide values demonstrated that the obtained oils are stable and suitable for biodiesel production.

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The in vivo evaluation of RNase-A@PbS QDs based on avian embryo as an animal model

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Key words: animal model, embryotoxicity, irritation potential, PbS QDs

Over recent years the field of nanomaterials, particularly quantum dots has accepted the chicken model as a rather useful one, a quick and cheap alternative to evaluating embryotoxicity of new nanoparticles with respect to traditional animal models. Lead sulfide quantum dots (PbS QDs) have been widely investigated for biomedical imaging applications due to their favorable optical properties. The chicken embryotoxicity screening test (CHEST) and the chicken chorioallantoic membrane (CAM) are widely used models in medical research and fulfil the requirements laid out in the 3 R's principles, also with regard to similar development with mammals. This study combines evaluating the embryotoxic effect using the chicken embryotoxicity screening test (CHEST) and irritation potential evaluated with the Luepke grading system of the different administered concentrations of PbS QDs (10%, 25%, 50%, 100%). The results demonstrated that the administration of QDs different concentrations at early stage of development (embryonic day 4) did not affect the body weight of chicken embryos or the weight of selected organs (liver, heart). A mild decrease in body and organ weights was observed at 25% PbS QDs. The mortality of chicken embryos was increased with rising PbS QDs concentrations, and the LD_{50} was determined to 117 µl /egg. In 100% PbS QDs group as an extreme-dose condition was observed the 56% of mortality 5 days after the administration. Furthermore, the irritation potential suggests a slight effect at all tested concentrations, with a vasodilation like the main effect on the 9th embryonic day. The evaluation of the results thus indicates/confirms the biosafety of the tested PbS QDs regarding to the developing organism, particularly at doses relevant to biomedical imaging applications.
This work was supported by the Slovak Research and Development Agency under the Contract no. SK-CN-23-0017.

Posters: Risk management and process safety

Enhancing the safety of chemical processes using a dynamic digital system

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Key words: chemical process safety; Aspen HYSYS; dynamic simulation; nonlinearity; multiple steady states; Morris method

The work is focused on verifying the possibilities of using Aspen HYSYS for the analysis of steady-state and dynamic system behavior, on assessing its practical applicability for modeling a chemical process from the viewpoint of hazardous states, and at the same time on evaluating whether the use of a commercial simulation program can accelerate calculations and reduce the time required for a more extensive safety analysis. Part of the solution was the development of a mathematical model in MATLAB, which served as a reference and comparative basis for the results obtained in the commercial simulation environment Aspen HYSYS. In Aspen HYSYS, models of a CSTR, a CSTR with an external heat exchanger, and subsequently a CSTR approximated by a PFR model with heat exchange were developed step by step. In the case of the simple CSTR model, it was shown that Aspen HYSYS does not allow a sufficiently realistic description of heat transfer between the reaction mixture and the cooling medium, since heat removal could only be defined by a fixed heat duty. Therefore, a CSTR model with an external heat exchanger was created, although it enabled cooling by means of cooling water, it did not fully correspond to the behavior of an ideally mixed reactor. For these reasons, a PFR model was finally selected and configured to approximate CSTR behavior as closely as possible, while also providing a more suitable description of heat transfer and showing very good agreement with the reference MATLAB model. Using this model, continuation diagrams of selected input parameters were analyzed under steady-state conditions, namely reactant flow rates, inlet temperatures, cooling-medium flow rate, and cooling-medium inlet temperature. The results showed that all analyzed parameters exhibit nonlinear behavior accompanied by the occurrence of multiple steady states. Since the steady-state calculations indicated the sensitivity of the system to changes in input parameters, the next part of the analysis focused on system behavior in the dynamic regime. In the dynamic regime, attention was paid to the system response to deviations from the operating point, as well as to the effect of their duration on the system's ability to return to the original steady state. The simulations confirmed that the dynamic model in Aspen HYSYS is able to reliably describe system behavior on individual solution branches, although transitions between the individual branches of steady states could not be captured reliably. The final step of the nonlinearity analysis consisted in the use of the Morris method as a tool of global sensitivity analysis. Based on this method, the input parameters with the most significant influence on the model outputs were identified, with the flow rates of both reactants showing the strongest nonlinearity. The obtained results indicate that a model-based approach in Aspen HYSYS makes it possible to analyze the safety aspects of a chemical process reliably and at the same time more time-efficiently, which is particularly important when modeling larger-scale chemical plants.

The significance of hydrogen concentration monitoring in primary coolant circuits

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Key words: hydrogen determination; primary circuit; chemistry control; coolant radiolysis

To keep nuclear reactor's cooling loop as safe as possible, the production of corrosive species should be reduced during the coolant radiolysis. In the literature, several mathematical models exist to calculate the corrosive species concentration and to predict their decrease in dependence on hydrogen dosage into the primary coolant. None of the models, however, describes reliably the real situation and the calculated concentrations of individual species differ from the measured process values even by one order, as we show in the first part of this contribution. Therefore, the reliable way for primary circuit chemistry control is the process measurement of the concentration of as many species as possible. The most important species determining the primary circuit chemistry is hydrogen. Therefore, we deal with the hydrogen sensor development because there is a lack of really sensitive hydrogen sensors on the world market. This year, after reporting on the process tests in recent years, we report on the H-meter device optimization both from the viewpoint of the time span of its usage (service period) and from the viewpoint of its geometrical arrangement. The main results of the last period of H-meter development are the incorporation of recalibration system (HW and SW) and a consequent reduction of the device volume by 1/3.

Posters: Environmental chemical engineering

Biochar as an Effective Adsorbent for the Removal of Heavy Metals from Water

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Key words: heavy metals, biochar, wastewater, adsorption, temperature

Heavy metals in aquatic environments pose a significant environmental and health risk even at low concentrations. Lead (Pb), originating mainly from industrial sources, is particularly associated with neurological disorders. Among the effective removal methods, adsorption is considered especially efficient at low contaminant concentrations.
This study focuses on the use of biochar as an adsorbent for lead removal. Biochar was produced from plum pits via pyrolysis at temperatures ranging from 300 to 800 °C and subsequently characterized using BET analysis. Adsorption experiments were conducted at pH 5, where lead predominantly exists in the Pb^{2+} form.
The results confirmed that increasing pyrolysis temperature leads to a higher specific surface area of biochar, resulting in improved adsorption efficiency. Biochar produced at 300 °C achieved an efficiency of approximately 43%, while materials prepared at 700–800 °C reached efficiencies of up to 80%. Pyrolysis temperature was thus identified as a key factor influencing the adsorption properties of biochar.

Biochar-supported materials for lithium recovery: Comparison of ion-imprinted polymers, lithium ion sieves, and MnO_x composites

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Key words: lithium recovery, biochar, hybrid materials, MnO_x, ion-imprinted polymers, lithium ion sieves

Abstract

This study evaluates biochar-supported materials for Li^+ recovery, including ion-imprinted polymers (IIP), lithium ion sieves (LIS), and MnO_x-modified biochar. Hybrid materials were prepared using wood chip biochar (WCB) and walnut shell biochar (WSB) as supports and characterized by ATR-FTIR and SEM-EDX. Despite the successful incorporation of MnO_x phases and imprinted polymers, both LIS and IIP systems showed only negligible Li^+ adsorption (≤0.011 mg/g). The limited efficiency of LIS is attributed to acid activation in 0.5 M HCl, probably causing partial MnO_x destabilization. IIP materials showed negative sorption due to incomplete template removal and Li^+ release from the polymer matrix. On the contrary, MnO_x-modified biochar (WSB-IM) showed measurable adsorption, with an experimental Q_{max} reaching 1.28 mg/g. Adsorption was better described by the Freundlich model (R^2 = 0.997), indicating heterogeneous surface interactions. However, strong competitive effects of Na^+ and Mg^{2+} reduced adsorption capacity to 0.083 and 0.068 mg/g, and to 0.02 mg/g in mineral water. These results suggest that the performance of Li^+ sorbents is governed not only by intrinsic selectivity but also by the stability and accessibility of the active phase, particularly in biochar-supported systems.

Comparison of different approaches for improvement of nanofiltration of industrial effluent

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Key words: Industrial wastewater, nanofiltration, pH regulation, wastewater treatment

Wastewater from resin production, particularly phenolic resins, is characterized by extremely high levels of organic pollutants such as phenol, formaldehyde, and solvents. These effluents often exhibit high chemical oxygen demand (COD), toxicity and low pH, making them resistant to conventional biological treatment alone. Current treatment strategies emphasize a multi-stage approach to meet discharge standards and promote water reuse**.** Phenol and formaldehyde can be recovered selectively through liquid-liquid extraction (LLE) using specialized extractants. The resulting stripping concentrates can be directly reused in the next resin production cycle. Resins could also be synthesized on-site by forming resol phenolic resins or mixed urea-formaldehyde resins within the treatment stream itself. This simultaneously purifies the water and produces a marketable technical product. Solvents can also be reclaimed using fractional distillation or vacuum distillation. Advanced membrane distillation and pervaporation offer lower-energy alternatives for breaking azeotropes and recovering pure solvents. Solid residues or concentrated organic fractions can be repurposed into wood-polymer composites or sodium phenolate. These materials could be used in construction and other industrial sectors. The aim of our work was theoretically compare three different approaches to tackle with a problem of industrial wastewater: i) Ca precipitation with CO_2, ii) Ca precipitation with Ca acetate and ammonium carbamate; and iii) Ca precipitation with $NaCO_3$. Effluent was pretreated by aerobic biological wastewater treatment plant and then proceed by nanofiltration, where $CaSO_4$ is deposited on membranes as a result of chemicals added in previous processes. With application of precipitation Ca should be removed before nanofiltration to prevent clogging. Average effluent flow was 2 m^3/h, COD 20,000 mg/L, pH 6-8, concentration of the sulphate 1000 mg/L and concentration of the Cl^- 100 mg/L. To compare optimal processes, Life Cycle Assessment (LCA) was calculated using SimaPro model to compare environmental impact based on 13 environmental parameters for all processes (carbon footprint, ozone depletion, Etc.)

Comprehensive Characterization of Steel Furnace Slag and Assessment of Pre-Treatment Efficiency for Wet Magnetic Separation: towards the valorization and reuse of magnetically isolated fractions

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Key words: slag, wet magnetic separation, efficiency, characterization, pre-treatments.

Global steel production has shown continuous growth over time, largely driven by industrialization and urbanization processes. Pyrometallurgical processing of mineral ores produces a large volume of metal-bearing waste (slag). Due to the presence of magnetic iron oxides, these by-products could not only be reused in steel production but also aid in the generation of novel materials. In this study, a steel furnace slag was fully characterized and magnetically separated considering 1 and 2-hour calcination at three different temperatures (400, 600 and 800 °C) and ultrasonication as pre-treatments. The characterization of the raw slag and the products after the pre-treatments allowed us to evaluate their morphology, phase composition, magnetic response and hyperfine parameters. Altogether, this information enabled the assessment of the effectiveness of the pre-treatments on improving the wet magnetic separation process. XRD results of treated samples showed a reduction in the intensity of the peaks corresponding to the main iron oxide phase on the raw slag (wüstite) and an increase in the magnetite reflections, considering both holding times during thermal treatments. Mössbauer spectroscopy confirmed that the increment in the pre-treatment temperature to 600 °C and 800 °C, either during 1 or 2 hours, generated a principal iron phase transformation into magnetite. The saturation magnetization value determined for the raw slag was 2.7 Am^2/Kg, while the products of the thermal treatments presented values of 2.7, 5.7, 10.0 Am^2/kg and 2.9, 6.7, 9.6 Am^2/kg for samples calcined at 400, 600, and 800 °C during 1 and 2 hours, respectively. These results indicate that the pre-treatments yielded a material that is more responsive to an external magnetic field. In fact, the processes performed at 600 °C and 800 °C improved the segregation of magnetic phases, resulting in recovery mass percentages of around 80%, which are considerably higher than those obtained from the wet magnetic separation of untreated slag. These findings positioned this by-product as a suitable candidate for a phase transformation, boosting its magnetic response and improving the efficiency of separation. The assayed pre-treatments generated favorable changes in the slag, increasing its magnetite content and consequently its magnetic response, which helped to improve the yield during the magnetic separation.

Design and development of a functionalized biochar sorbent with 2-(hydroxymethyl)-12-crown-4 ether for selective Li separation

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Key words: lithium, functionalized biochar, separation, crown ether, selective sorption

Abstract

Sorption is a promising separation technique for lithium recovery from aqueous streams and industrial liquid waste; however, its efficiency is often limited by the presence of competing ions. In this study, a selective sorbent was developed using cherry pit–derived biochar as a low-cost precursor. Biochar produced via slow pyrolysis at 500 °C (BC) was chemically functionalized with 2-(hydroxymethyl)-12-crown-4 ether to enhance Li^+ affinity, yielding the modified sorbent (F-BC). The physicochemical properties of the materials were characterized by FT-IR spectroscopy to confirm successful surface modification. Batch sorption experiments revealed a ~20-fold increase in lithium sorption capacity of F-BC relative to pristine biochar. Selectivity tests performed in multicomponent systems demonstrated preferential Li^+ uptake over competing monovalent (Na^+, K^+) and divalent (Ca^{2+}, Mg^{2+}) ions, indicating favorable ion-recognition behavior of the functionalized surface. The enhanced performance is attributed to the specific complexation of Li^+ with crown ether moieties. The results suggest that F-BC is a viable candidate for selective lithium recovery in complex aqueous matrices, with potential applications in resource recovery and wastewater treatment.

Electricity Consumption and Energy Efficiency Trends in Large Municipal Wastewater Treatment Plants in Slovakia

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Key words: wastewater treatment plants, Slovakia, electricity consumption, specific energy demand

Abstract

This study presents a comprehensive evaluation of electricity consumption in 57 large municipal wastewater treatment plants (WWTPs) in Slovakia based on detailed operational data for the year 2024. The analysed facilities represent approximately 3.0 million population equivalents (p.e.), corresponding to about 76% of the total pollution load treated in Slovak municipal WWTPs. Electricity demand was assessed using two key indicators: energy consumption per volume of treated wastewater (kWh/m^3) and per population equivalent per year (kWh/p.e.year). These indicators were further analysed in relation to plant size, influent characteristics and the presence of on-site energy generation. The results show that electricity consumption ranged from 0.13 to 1.19 kWh/m^3, with an average value of 0.45 kWh/m^3. When expressed per population equivalent, values ranged from 18.12 to 133.57 kWh/p.e.year, with an average of 49.33 kWh/p.e.year. A clear relationship was observed between influent organic load (BOD_5 concentration) and electricity consumption, reflecting increased aeration energy demand for higher organic pollution levels. While the kWh/m^3 indicator is widely used, the kWh/p.e.year metric proved more suitable for inter-plant comparison, as it better accounts for differences in influent strength. A significant inverse relationship between plant size and specific electricity consumption was identified when using the population-based indicator, confirming that larger WWTPs benefit from economies of scale. This trend was less pronounced when using the volumetric indicator. Despite extensive modernization efforts in the Slovak wastewater sector since 2011, average electricity consumption has remained relatively stable. This suggests that increased treatment requirements and more advanced process configurations have offset potential energy savings. In terms of energy production, 31 of the 57 Slovak WWTPs had on-site electricity generation, mainly through combined heat and power (CHP) units and photovoltaic systems. The

average electricity production reached 8.7 kWh/p.e.year, with a maximum of 24.4 kWh/p.e.year. Plants with energy generation achieved an average self-sufficiency rate of 22.1%. The findings provide a robust national benchmark for electricity consumption in WWTPs and offer valuable insights for future optimization. They also contribute to assessing progress toward energy efficiency and energy neutrality targets outlined in Directive (EU) 2024/3019.

Acknowledgement

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Greenness and whiteness evaluation of *ex-situ* small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry for *on-site* battery operated micro-solid phase extraction of Cu(II), Cd(II), Pb(II) and Zn(II) from river water

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Keywords: greenness degree, whiteness degree, AGREEprep metric, RGB 12 algorithm, *on-site* micro-solid phase extraction, *ex-situ* capacitively coupled microplasma optical emission spectrometry determination

The study presents the greenness and whiteness evaluation of an *on-site* battery-operated micro-solid phase extraction (μ-SPE) of Cu(II), Cd(II), Pb(II) and Zn(II) from river water using dithizone-functionalized C18 cartridges and determination by *ex-situ* capacitively coupled microplasma optical emission spectrometry after vaporization from a small-sized electrothermal vaporization device of Rh coiled filament. The assessment was carried out using two of the most objective tools freely available online, namely the AGREEprep metric, used for greenness evaluation of the sample preparation procedure, and the RGB 12 algorithm, used for redness, greenness, blueness and whiteness characterization of the whole analytical determination. The AGREEprep metric highlighted a greenness score of 60%, mainly due to the *on-site* sample processing, energy-free operation due to the battery-operated experimental setup, reusability of the dithizone-functionalized C18 cartridges and fully miniaturized instrumentation. The RGB 12 algorithm, on the other hand, provided redness/greenness/blueness/whiteness degrees of 92/68/91/84%, respectively, due to the substantial improvement of the limits of detection by the high preconcentration factors of the analytes, cost-efficiency of miniaturized instrumentation, time efficiency by simultaneous analysis and operational simplicity. A comparative assessment with conventional bulky laboratory instrumentation, including graphite furnace atomic absorption spectrometry and inductively coupled plasma optical emission spectrometry, revealed lower greenness (53% and 41%) and whiteness scores (73% and 67%). Overall, the microplasma-based method demonstrated a highly sustainable and efficient alternative for trace metal analysis in environmental water samples.

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High Entropy oxides as catalysts in advanced oxidation processes for wastewater treatment

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Key words: Catalytic systems, high entropy oxides, micropollutants, wastewater treatment

High-entropy oxides (HEOs) are a group of relatively new oxide materials having at least five cations, and consequently a high degree of structural disorder. These five different metal oxide components are simultaneously contained in a single-phase crystal system, whereby the metal ions can have completely different ionic radii, which leads to a so-called structural lattice distortion effect. The distorted lattice (or strain in the crystal structure) is the obstacle to dislocation movement, which increases the strength and reduces the ductility of the finished material. HEO materials are also attributed to the so-called cocktail effect, where the different elements act synergistically and therefore also exhibit excellent catalytic properties. They have a great potential for application in various fields, including catalysis, electrochemical energy transformation and the environment. Various catalysts for catalytic ozonation, including homogeneous and heterogeneous catalysts, such as metal ions, metal oxides, and carbon-based materials are recently being investigated in terms of advanced oxidation processes. Two new innovative approaches for HEO synthesis were presented: combustion synthesis and solvent deficient method. The composition and morphology of resulting HEO products were analyzed using XRD powder diffraction method and FE-SEM equipped with EDS detector. The aim of our study was to synthesize rock-salt HEO $(Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2})O$ and test its efficiency as catalyst in advanced oxidation processes based on Fenton reaction and ozonation. Batch experiments were conducted in laboratory scale and treatment efficiency of methylene blue as a model compound was studied using absorbance measurements. Toxicity of the leachates of HEO was also determined using *Lemna minor* to assess its impact to aquatic environment. It was confirmed, that investigated HEO could be used as a catalyst in oxidative treatment of micropollutants but its efficiency is strongly dependent upon reaction conditions.

Immobilized PET-degrading enzymes for microplastic control

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Key words: polyethylene terephthalate (PET) degradation, nanoPET, leaf-branch compost cutinase (LCC)

The accumulation of polyethylene terephthalate (PET) represents a major environmental threat due to its durability and widespread use. Enzymatic hydrolysis mediated by PET-degrading enzymes, particularly leaf-branch compost cutinase (LCC), offers a sustainable approach for PET depolymerization into its monomers: BHET, MHET, TPA, and EG.[1,2] In this study, two recombinant LCC were successfully produced in *E. coli* Rosetta pLysS using a pET-21a(+) vector. For process evaluation, two methods (HPLC and UV-Vis spectroscopy) were optimized. The golden-standard LCC-ICCG variant and one in-house developed mutant (LCC-ISN) were tested for nanoPET degradation. Some nanomaterials were tested as support for native and mutant enzymes immobilization. [3,4]

The use of smaller concentrations of enzyme was proven more efficient for PET hydrolysis in the first 24 hours. The in-house produced mutant LCC-ISN has a higher activity in degrading nanoPET in the first 24 hours as compared to the golden-standard LCC-ICCG.

Magnetic nanoparticles covered with amino-silanes or with Chitosane, further functionalized with EDTA anhydride and Co^{2+}, were tested as support for the enzyme variants immobilization, and the resulted biocatalysts were efficient for the nanoPET degradation.

The immobilization method and the use of the in-house mutant represent a new approach towards resolving the ongoing efforts to develop enzyme-based solutions for PET biodegradation and sustainable plastic recycling.

Acknowledgements

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Impact of Environmentally Relevant Antibiotics and Heavy Metals on Anaerobic Digestion of Waste Activated Sludge

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Key words: antibiotics, heavy metals, biogas production, methane, volatile fatty acids

Anaerobic digestion is a key technology for sewage sludge stabilization and renewable energy recovery in the form of biogas. However, the increasing presence of emerging contaminants, such as antibiotics and heavy metals, in wastewater streams raises concerns regarding process stability and efficiency. These compounds, even at environmentally relevant concentrations, may interfere with microbial activity. Additionally, their co-occurrence may lead to complex interactions, potentially resulting in synergistic or antagonistic effects, as well as contributing to the co-selection of antibiotic and metal resistance.

This study investigates the effects of clarithromycin and copper and zinc on anaerobic digestion of waste activated sludge. Batch experiments are conducted using anaerobic reactors operated under controlled conditions. The tested compounds are introduced both individually and in combination. The applied concentrations reflect levels typically reported in wastewater and sludge, ensuring environmental relevance.

The results indicate that the impact of antibiotics and heavy metals on anaerobic digestion of waste activated sludge depends strongly on the type of metal and its concentration. The presence of clarithromycin alone did not result in substantial changes in biogas production compared to the control, suggesting limited inhibitory effects at environmentally relevant levels. However, clear differences were observed when antibiotic was combined with metals. In particular, systems containing copper exhibited a dose-dependent response: lower concentrations were associated with enhanced biogas production (326 mL CH_4/gVS), while higher concentrations led to a pronounced decrease in process efficiency (76 mL CH_4/gVS. This may be linked to the dual role of copper as both an essential trace element supporting microbial enzymatic activity and a toxic compound at elevated levels. In contrast, zinc-containing systems showed more moderate effects, with no clear inhibitory trends observed under the tested conditions. The results suggest that anaerobic microbial communities demonstrate a relatively high resilience to low-level contaminant exposure, while combined stress can significantly influence process performance. This work was supported by the Polish National Science Center (Project No. 2024/55/B/NZ9/00815).

Influence of waste feedstock composition on thermo-catalytic conversion products

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Key words: gasification, waste feedstock, mixed waste treatment

Waste generation has become a significant challenge, leading to environmental, health, and economic impacts. Waste streams that are unsuitable for material recycling can instead be utilized for energy and material recovery. Significant issue with treatment of the waste feedstocks is their heterogeneous composition, which varies on a daily basis. This work investigates effect of feedstock composition on the gasification product properties, with the aim to achieve constant product properties from feedstocks with variable composition. Feedstock samples containing different ratios of refuse derived fuel (RDF), anaerobic digestion digestate, lignocellulosic biomass (sawdust) and mixed plastics were prepared and pelletized. All the samples have similar key parameters (heating value, ash content, contaminant concentrations etc.), even though ratios of their components vary. Each sample was gasified in a continuous three-stage pyrolysis/split product reactor. In the first stage, pyrolysis took place in the screw reactor at 650°C. Pyrolysis char entered the second stage, where it was gasified at 800°C in the presence of air. Produced gas entered third stage, where catalytic cracking occurred at 850°C in the presence of 3 wt.% nickel on activated carbon catalyst. Distribution of the gasification products from different feedstocks was similar, while yield of produced gas was the highest among the products. Main components of the gas were H_2, CO, CO_2, CH_4 and C_2H_x hydrocarbon fraction, which resulted in gas with high heating value. Gas was contaminated with high amounts of tar despite the use of tar-cracking catalyst, as well as H_2S, COS and HCl originating from sulfur and chlorine present in feedstock. Solid product of the gasification (char) consisted of mainly ash and carbon. Yields of ash in this product were similar after gasification of different samples, meaning that variations in total char yield were caused by different carbon content. Overall product properties were similar to each other, even though they were produced by different feedstock samples. Achieving consistent product properties is important for waste treatment processes and ensures smooth operation of the gasification unit.

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Morphology-controlled crystallization of $Mg(OH)_2$ through ion-exchange membrane crystallization

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Key words: magnesium hydroxide, anion-exchange membrane, membrane crystallization

Brines generated during seawater desalination and other industrial processes represent a significant environmental issue due to their high concentration of dissolved salts. At the same time, these streams represent a potential source of valuable raw materials, including magnesium. Its recovery by conventional precipitation methods is often associated with co-precipitation of other substances, low product quality, and difficult separation of the resulting solid phase. A promising alternative is reactive membrane crystallization, in which the precipitating agent is separated from the brine by an ion-exchange membrane, thereby reducing the risk of product contamination while improving process control.

This work is focused on the recovery of magnesium in the form of magnesium hydroxide from model brines using hollow multi-fibre module equipped with anion-exchange hollow fibres. Sodium hydroxide, as the precipitation agent, was circulated inside the fibres, while the membrane module was immersed in a magnesium chloride solution. The transport of hydroxide ions through the membrane led to their reaction with magnesium ions and to the formation of $Mg(OH)_2$ precipitate. The study investigated the influence of operating conditions on both process performance and product morphology, with particular attention to reactant concentrations, solution volumes, volumetric flow rates, and packing density of the fibre bundle.

The morphology of the produced $Mg(OH)_2$ particles was evaluated by scanning electron microscopy, while the behaviour of the process was further interpreted using a mathematical model. The model consists of a system of ordinary differential equations solved in MATLAB describing mass-transfer and reaction phenomena in a two-compartment system separated by a single anion-exchange membrane.

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On-site battery-operated micro-solid phase extraction of Cu(II), Cd(II), Pb(II) and Zn(II) from river water followed by *ex-situ* small-sized electrothermal vaporization capacitively coupled microplasma optical emission spectrometry determination

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Keywords: micro-solid phase extraction, *on-site* river water processing, dithizone-functionalized C18 cartridge, capacitively coupled microplasma optical emission spectrometry

The development of analytical methods aligned with the principles of Green and White Analytical Chemistry for the determination of priority hazardous metals, such as Cd and Pb, remains a significant challenge due to their ultra-trace concentration levels and the need for highly sensitive yet sustainable methodologies. Thus, the aim of this study was the development of a battery-operated *on-site* micro-solid phase extraction (μ-SPE) system based on dithizone-functionalized C18 cartridges coupled with *ex-situ* small-sized electrothermal vaporization capacitively coupled plasma optical emission spectrometry (SSETV–μCCP–OES) for the simultaneous determination of Cd(II), Cu(II), Pb(II), and Zn(II) in river water. The μ-SPE procedure was optimized in terms of immobilized dithizone quantity on the C18 cartridge, sample pH and flow rate during preconcentration and eluent composition and volume. The accuracy (recovery and precision) of the method was evaluated by analyzing several water certified reference materials (CRMs), obtaining recoveries in the range 93–108%, and precision of 11–15%, respectively. The *ex-situ* optimized method was then applied for *on-site* river water processing, powered by a photovoltaic panel-charged battery, followed by *ex-situ* simultaneous determination of Cd(II), Cu(II), Pb(II), and Zn(II) using the fully miniaturized SSETV–μCCP–OES system, characterized by low power (15 W) and low Ar consumption (150 mL min^{-1}). The proposed approach provides a portable, energy-autonomous, and cost-effective alternative for sustainable ultra-trace metal monitoring in surface waters, compared to classical benchtop laboratory instrumentation.

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Sustainable LiOH Production by Bipolar Membrane Electrodialysis in a Closed-Loop Recycling Scheme

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Key words: lithium recovery, electrodialysis, bipolar membrane.

Global lithium demand has increased dramatically over the past two decades, driven mainly by Li-ion battery production. Despite the strategic importance of lithium, recycling rates of spent batteries remain very low, and no universal recycling route has been established. Hydrometallurgical recycling typically involves black mass production, acid leaching, purification of the leachate, and subsequent conversion of lithium into high-purity high-value products such as lithium hydroxide (LiOH).

This work focuses on valorization of a purified lithium stream by converting lithium sulfate (Li_2SO_4), commonly obtained after sulfuric acid leaching, into LiOH using electrodialysis with bipolar membranes (EDBM). Bipolar membranes enable in situ water dissociation, producing alkaline and acidic streams without the use of external chemical reagents. Produced LiOH can be subsequently crystallized and produced sulfuric acid can be directly recycled back to the leaching step, supporting a closed-loop concept. Because the conversion of the lithium salt leave purified water as the only remaining liquid phase, the process aligns well with Zero liquid discharge (ZLD) concept. Four different membrane types were investigated for LiOH production, evaluating specific energy consumption and the purity of the produced LiOH stream. Two membrane types enabled production of high-purity LiOH suitable for immediate crystallization while maintaining low energy demand. To intensify downstream processing, concentration steps were also investigated. Conventional electrodialysis was insufficient to reach saturation point, therefore membrane distillation was examined as an alternative, allowing additional concentration by utilizing waste heat.

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Waste biomass-to-electrode materials: biochar-based carbon for electrochemical flow systems

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Key words: biochar, electrodes, modification, green chemistry, ascorbic acid

The valorization of plant-based waste into functional carbon materials represents a promising route for integrating waste management with advanced material engineering. In this study, lignocellulosic residues—sunflower seed shells, beech wood sawdust, cereal straw, and Chinese silvergrass—were converted into biochar via slow pyrolysis at 750 °C under a controlled nitrogen atmosphere. The process conditions were selected to promote the development of porous carbon structures suitable for electrochemical applications. The produced biochars were characterized with respect to key physicochemical parameters, including specific surface area, micropore volume, surface chemistry (pH, point of zero charge), electrical conductivity, and ion exchange capacities. Based on these properties, electrodes were fabricated either from pure biochar or as composites with reticulated vitreous carbon (RVC) at mass ratios of 70:30 and 90:10 (RVC:biochar), enabling the tuning of structural integrity and electroactive surface properties. Electrode performance was evaluated in a continuous flow electrochemical system using chronopotentiometric detection of ascorbic acid as a model compound. Operational parameters, including current density and flow conditions, were optimized to ensure stable signal response and mass transport control. The composite electrodes exhibited linear response ranges of 18–500 mg L^{-1} (70:30) and 15–500 mg L^{-1} (90:10), with minimal sensitivity to electrolyte composition. Improved repeatability and signal stability were observed for the 90:10 configuration, indicating a favorable balance between conductivity and active surface area. Application to real samples (fruit beverages and vitamin supplements) confirmed the practical applicability of the developed system. The results demonstrate that thermochemically derived biochar from waste biomass can be engineered into functional electrode materials with competitive performance in flow electrochemical systems. This approach highlights the potential for scalable integration of biomass conversion processes with the production of value-added electrochemical components.

Posters: Process design and process intensification

Plasma-activated water: The Impact of Physicochemical Properties on its Antimicrobial Efficacy

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Key words: plasma activated water, reactive oxygen species, reactive nitrogen species, antimicrobial efficacy, organic impurities.

Plasma-activated water (PAW) is a novel and sustainable technology that has attracted considerable attention in various fields of application, including disinfection, due to its strong antimicrobial efficacy. PAW has already been proven effective against a wide range of microorganisms, including bacteria, biofilms, spores, yeasts, and even certain viruses. In contrast to most used disinfectants in veterinary medicine, which are based on chemical compounds, PAW does not contain any added chemical substances that could pose a risk to human or animal health and harm the environment.

PAW is produced when water is treated with plasma, an ionized gas. The chemical reactions that take place lead to the formation of reactive oxygen and nitrogen species (RONS), such as hydroxyl radicals (•OH), nitric oxide (NO) and peroxynitrite ($ONOO^-$), which typically have a half-life ranging from nanoseconds to a few seconds, as well as long-lived species such as hydrogen peroxide (H_2O_2), ozone (O_3), nitrite (NO_2^-) and nitrate (NO_3^-). Therefore, PAW is a dynamic system rather than a stable entity, in which short-lived reactive species continuously decay and transform into more stable compounds. Along with the resulting low pH and high oxidoreduction potential (ORP), these factors are considered the key contributors to PAW's antimicrobial activity. However, the efficacy of disinfectants depends on various factors. One of them is the presence of impurities in the environment, particularly those of organic origin. Therefore, in our future research we aim to address the antimicrobial efficacy of PAW against relevant microorganisms encountered in veterinary medicine in the presence of organic matter, while simultaneously evaluating its selected physicochemical parameters. Our study follows the standardized protocols used for testing the efficacy of commercial chemical disinfectants, which include assessing disinfectant efficacy in the presence of organic matter. This enables comparison with established chemical disinfectants and, at the same time, the standardization of the antimicrobial efficacy of this novel disinfectant. We will also attempt to identify the products formed in the process, as it is known that PAW induces the degradation of organic matter, which will also contribute to understanding of the environmental acceptability of this potential disinfectant.

The grinding process as a determinant of the chemical properties of freeze-dried fruits

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Key words: fruit, freeze-drying, grinding, chemical properties

Fruit are characterised by chemical properties that play a significant role in the functioning of the human body. Many fruits are available only at certain times of the year. For this reason, fruits are preserved, including through freeze-drying. Freeze-dried fruits are available on the Polish market in various forms, including whole fruit and those ground into grits or powder. The grinding process of freeze-dried fruit can alter the chemical properties of these products.

The study aimed to assess the effect of the grinding process on selected chemical properties of freeze-dried fruits. The research material consisted of freeze-dried strawberries, raspberries, cherries, blueberries, blackcurrants, and blackberries, in whole form and as grits and powder. They were purchased online.

Chemical properties were determined based on the determination of water content and activity, total anthocyanin content, vitamin C, total polyphenolic compounds, and the degree of free radical reduction. The obtained results were statistically analysed. The effects of species and the grinding process on the analysed chemical parameters in freeze-dried fruits were determined using multivariate analysis of variance (ANOVA). The significance of differences between the study groups was tested using Tukey's test. Relationships were considered statistically significant at $p < 0.05$.

The study showed that whole freeze-dried fruits had lower water content and activity, higher levels of anthocyanins, vitamin C, and polyphenolic compounds, and a greater ability to reduce free radicals than ground freeze-dried fruit. Grinding into grits or powder significantly reduced the chemical properties of the analysed products. Furthermore, significant differences in the chemical properties of freeze-dried fruits were observed across species.

Posters: Digitalization and process control

A Practical Approach to Anomaly Detection in Industrial Data

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Industrial processes are usually continuously monitored using two types of measurements, online sensors (low-fidelity measurements, LF) and laboratory analyses (high-fidelity measurements, HF). Low-fidelity measurements provide frequent but potentially noisy, inaccurate, or fault-affected data, while high-fidelity measurements are less frequent but are considered to accurately represent the true process values. Comparing LF and HF data may reveal big discrepancies between these measurements, which can indicate the presence of anomalies. Anomalies are patterns in a dataset that deviate from general trends and expected behaviour [1]. Their detection is critical for early identification of sensor faults, maintaining data quality and reliability of models. Corrupted measurements may result in failure to achieve desired process targets.

For the purpose of this work, data are used from the alkylation unit at Slovnaft, a.s. Since the available dataset contains a large number of process variables, we select most relevant features using correlation analysis and Partial Least Squares (PLS) regression. We use the resulting feature subset as input to anomaly detection models. To evaluate models performance, we compute confusion matrices using ground-truth anomalies and predicted anomalies. A multi-fidelity model, described in [2], is used to define the ground-truth anomalies. This model uses a simple residual-correction approach combining a dynamic LF predictor with a Gaussian Process correction learned from HF data. To define predicted anomalies we use Density-Based Spatial Clustering of Applications with Noise (DBSCAN), Ordinary Least Squares (OLS) regression, and Gaussian Process Regression (GPR). We optimize anomaly detection models parameters using the Nelder-Mead method, targeting the best balance between detection sensitivity and false alarm rate.

The results indicate that each of the considered methods provides a different perspective on the data structure and types of deviations. When comparing regression methods, OLS generally achieves better performance than GPR, suggesting that more complex nonlinear methods do not provide additional benefits for this type of data. The proposed framework contributes to improving measurement reliability and may support early detection of sensor faults.

Key words: Anomaly detection, Confusion matrix, Optimization, Soft sensors, Laboratory analyses

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A Simplified Framework for Process Model Development in Industrial Simulation Environments

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Industrial process systems are inherently complex, and detailed first-principles models or advanced control approaches are often difficult to implement and maintain in practice. This is particularly evident in alkylation units, where strong interactions, unmeasured disturbances, and operational variability limit the applicability of highly detailed models and complicate their long-term use in industrial environments.

This work proposes a framework for process model development based on a reduced set of process variables. The variable selection combines Principal Component Analysis (PCA), Partial Least Squares (PLS), LASSO regression, and stepwise regression to identify relevant variables from the available measurements. These methods are used to evaluate variable importance, collinearity, and contribution to the dominant process variability. The selection is then refined using process knowledge, where variables are assessed with respect to their physical meaning, measurement reliability, and availability in real operation. Variables that are statistically relevant but operationally unreliable or redundant are excluded or replaced by more suitable alternatives.

A steady-state model is constructed in gPROMS ProcessBuilder and AVEVA Process Simulation to represent the main unit operations and their interactions. The model is implemented using predefined process blocks that encapsulate the governing equations, rather than coding the model directly from first principles. The model captures the key process relationships at the unit level and enables systematic analysis of process behavior under varying operating conditions. The simplified structure avoids detailed kinetics and secondary effects, focusing on a stable and interpretable representation of the system.

The model is further used to analyse the influence of the selected variables on the system response and to verify that the reduced variable set is sufficient to describe the dominant system trends without loss of essential process information. The results confirm that the selected variables, together with the simplified model structure, provide a consistent and physically meaningful description of the main process behavior under real industrial constraints.

Key words: Feature selection, Process simulation, Mass-balance modeling.

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Batch Crystallisation Control Optimisation Using In-Line Monitoring and External Dynamic Nucleation Control

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Key words: crystallization, process analytical technology, process control, direct nucleation control, optimisation, crystal size distribution

Batch production remains widely used in the manufacture of fine chemicals and active pharmaceutical ingredients, mainly due to relatively small production scales and the diversity of target compounds. Crystallisation plays a decisive role, as it directly determines the properties of the final product.

This work presents the development and experimental validation of a prototype system designed to enhance crystallisation control through active nucleation control. The proposed solution integrates a modified crystalliser design with an external dissolution unit, enabling real-time control of the crystal population during operation.

A central feature of the system is continuous monitoring using in-line microscopy, combined with advanced image processing techniques supported by machine learning. This setup provides real-time information on crystal size distribution and process dynamics, forming the basis for closed-loop control.

The control strategy relies on process analytical technology (PAT), employing an advanced algorithm to adjust operating parameters in response to the current system state. This allows rapid corrective actions, resulting in improved product consistency and a reduced risk of off-specification material.

An experimental setup was assembled by adapting an existing internal DNC system with readily available and cost-effective components. A linear cooling experiment was first conducted to establish a reference case and define the expected particle count range. Subsequent experiments focused on increasing crystal size, demonstrating that process optimisation could be achieved within only a few experimental runs.

Inventory Monitoring in a Petrol Refinery via Data Reconciliation

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Key words: data reconciliation, mixed integer quadratic programming, optimisation problem, neural network

A typical inventory infrastructure in a refinery consists of a multitude of interconnected technological blocks with an extensive network of liquid storage tanks. Although measurements of input and output flows to some of these blocks and tank levels might be available, the precise flows to, from, and between individual storage tanks are not necessarily directly metered.
The goal of this work is to design a data reconciliation system coupled with mass balance to estimate the incoming, interconnecting, and outflowing streams for product storage tanks in the Slovnaft refinery, an industrial partner. We use mixed-integer quadratic programming (MIQP) to mathematically formulate the reconciliation problem using all known connections between tanks and physical laws, such as mass balances. The advantage of this method is the inclusion of binary variables, which naturally allows us to model behaviours where a stream can either enter a tank or not, and the outflow from a tank can enter only one specific block stream. This was implemented using YALMIP in MATLAB, specifically the Gurobi solver.
Subsequently, we used the optimisation results to train a feedforward neural network in order to achieve similar results in reduced central processing unit (CPU) time for real-time reconciliation. The neural network was also implemented in MATLAB.
The results showed that the neural-network-based optimiser was able to find the solution successfully for 98% of the given data, significantly lowering the measurement noise. The neural network model achieved high accuracy, with a correlation coefficient of 0.9982, and generated solutions 300 times faster on average than the optimiser.
In conclusion, this solution radically improves the accuracy of refinery monitoring, detects systematic errors, and demonstrates that neural networks are suitable tools for the use in real-time optimisation.

Acknowledgements: This work is funded by the EU Horizon Europe under the grant scheme NextGenerationEU projects no. 09I0103-V05-00002 and 09I01-03-V04-00024. RP also acknowledges the Scientific Grant Agency of the Slovak Republic under the grant 1/0263/25.

Robust Stabilization of Discrete-Time Switched Systems with Application to a CSTR

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Key words: Model predictive control, Input-to-state stability, Stabilization, Switched systems, Continuous stirred tank reactor

This work addresses the robust control of discrete-time switched systems subject to bounded disturbances and hard state and input constraints. To demonstrate the applicability of the proposed theoretical results, the modal dynamics of a continuous stirred tank reactor (CSTR) are considered as a motivating example. The combined presence of switching, disturbances, and constraints significantly complicates the control design and necessitates systematic guarantees of stability and robustness. Initially, mode-dependent state-feedback controllers are designed using linear matrix inequality (LMI) based techniques along with multiple Lyapunov functions. Under an average dwell-time switching framework, sufficient conditions are derived to guarantee exponential stability of the switched system in the absence of disturbances. These stability results are then extended to the case of bounded disturbances, where input-to-state stability is established, ensuring that the system states remain bounded for all admissible switching signals. Based on the obtained stability analysis, a tube-based robust model predictive control (MPC) scheme is developed for constrained switched systems. The control input is decomposed into a stabilising feedback component and an optimised nominal control component. A robust positively invariant set is constructed to handle the effect of disturbances and to ensure robust satisfaction of state and input constraints. Furthermore, recursive feasibility of the proposed predictive control problem is also ensured.

Acknowledgments: This work is funded by the European Commission under the grant scheme NextGenerationEU projects no. 09I0103-V05-00002 and 09I01-03-V04-00024. RP also acknowledges the Scientific Grant Agency of the Slovak Republic under the grant 1/0263/25. BK acknowledges the support provided by an internal young STU grant.

Technical Optimization Techniques for Eliminating Systemic Errors in Data for Digital Construction of Bread Using Image Analysis

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Key words: Image Analysis, Baking Industry, Energy Efficiency

Regarding a scientific knowledge of baking on industrial scale, qualitative information is vast, allowing for high quality products. Quantitative side is, however, left to be desired. Since the latter is what's required for optimization for energy efficiency, this work is a part of an aim to measure and eventually describe physical phenomena before and during baking. The work mentions only one of those variables – measurement of bread dimensions.
Measuring shape and volume changes of a bread before and after baking poses a unique challenge. Measurement has to be accurate and non-destructive as this determines the initial conditions in mathematical modelling. It must be performed in a quick succession, since any delays between proofing and baking changes the end quality of product and drifts away from the real process. Image analysis from pictures taken by camera provides an inexpensive and intuitive way to resolve such intricacies.
Image analysis is performed by taking at least three pictures with a reference of a known length within the picture. Since 2D images inherently provide limited information, the first requirement to achieve desired accuracy is to make sure that the reference is aligned with the plane of view, on which a measured dimension is determined. The second source of error comes from an inability of a camera to see parts of the intersection of measured solid due to perspective or the shape of the obstruction from the solid itself. In given conditions, even with the well-adjusted reference, the relative errors while measuring samples of a length 30 cm can be as high as 10 %.
This work showcases a setup and an apparatus to compensate for the limitations of the camera – it shows a plane of view for a reference and provides an indirect way of outlining the intersection of the sample. The apparatus tested on both laboratory and real-process conditions. The latest iteration showcases relative errors reaching below 1 %. The data can then be used to validate mathematical models of heat transfer in the dough/bread which are then utilized to optimize external conditions to achieve energy savings while maintaining overall quality of the bread.

[Chtěl jsem připsat, že by se hodil i obrázek, ale vidim, že na SSCHE 2026 stránkách chtěji abstract fo 400 slov only. Možná bysme mohli splodit i fulltext, co? Tematika obrazové analýzy je obecná, mohlo by to zajímat vícero lidí – tím bysme to i mohli uvést...]

Formatted: Czech

Posters: Separation processes and transport phenomena

Comprehensive experimental characterization of NeXRing #0.7 random packing

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Key words: Mass-transfer characteristics, Hydrodynamic performance, NeXRing packing

Random packings remain a key element of industrial absorption columns and gas-liquid contactors, where further improvements in hydraulic performance and mass-transfer efficiency are essential for reducing energy consumption while maintaining high process intensification. Among recent developments, the NeXRing packing family has attracted increasing industrial interest due to its advanced geometry, which enhances liquid distribution, lowers pressure drop, and increases effective interfacial area in comparison with conventional random packings. However, despite its practical relevance, open-literature experimental data for NeXRing packings, particularly for small-size elements, are largely unavailable.

This contribution presents a comprehensive and original experimental characterization of the hydraulic and mass-transfer properties of NeXRing #0.7 random packing under absorption operating conditions. To the authors' knowledge, this study provides the first complete publicly available dataset for this packing size. Hydraulic behaviour was investigated by pressure-drop measurements in an air-water system over a wide range of gas and liquid loads. Mass-transfer performance was evaluated using three well-established absorption systems: oxygen desorption from water to determine the liquid-side volumetric mass-transfer coefficient ($k_L a$), chemisorption of SO_2 into aqueous NaOH for the gas-side volumetric mass-transfer coefficient ($k_G a$), and chemisorption of CO_2 into aqueous NaOH to quantify the effective interfacial area (a). All mass-transfer characteristics were obtained using the subtraction method in order to eliminate end effects. Experiments were conducted in an atmospheric column with an inner diameter of 0.3 m, using packed-bed heights between 0.42 m and 1.3 m. The resulting experimental data were used to determine the hydraulic parameters (C_S, C_{Fl}, and $C_{P,0}$) and the mass-transfer parameters (C_L and C_V) of the Billet and Schultes (1999) model. The newly identified model parameters enable a reliable and validated description of NeXRing #0.7 performance, providing a solid basis for the design, comparison, and scale-up of absorption equipment utilizing this packing.

Electrodialysis for Zero Liquid Discharge: From Concept to Industrial Scale

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Key words: ZLD, electrodialysis, homogeneous, ion-exchange membranes,

Increasing environmental pressures, stricter regulatory frameworks, and rising costs of wastewater disposal are accelerating the adoption of advanced treatment technologies across industrial sectors. Zero Liquid Discharge (ZLD) has emerged as an effective strategy for minimizing wastewater generation while maximizing water reuse and resource recovery, particularly in the European Union, where environmental policies promote sustainable water management and reduced industrial emissions.

Among available technologies, membrane processes, especially electrodialysis, offer an energy-efficient alternative to conventional thermal methods for desalination and concentration of industrial streams. However, operation at high concentrations remains challenging due to reduced concentration gradients, back diffusion, scaling risks, membrane damage (burning), and decreased current efficiency caused by parasitic currents.

This work presents the development of an industrial-scale electrodialysis module tailored for ZLD applications. Based on laboratory evaluation of ion-exchange membranes, FUJI Type 12 membranes were selected due to their superior performance in achieving high concentrations. Analysis of their properties and module geometry showed that, to maintain current efficiency above 75%, a conventional single-stage design would be limited to approximately 150 membrane pairs, which is insufficient for industrial-scale operation.

To address this limitation, a multi-stage module was designed, consisting of four electrically and hydraulically independent stages separated by intermediate plates with bipolar electrodes. This configuration enables improved current distribution and reduction of parasitic losses. Experimental results demonstrated stable operation, achieving a maximum concentration of 230 g/L Na_2SO_4 with a current efficiency of 87%, confirming the suitability of the proposed design for ZLD applications.

Acknowledgement: This work was carried out in the frame of the IP project (Decision Nr. 6/2023) supported by the Czech Ministry of Industry and Trade. The project utilizes Membrane innovation centre infrastructure.

Evaluation of MellapakPlus 252.Y: pressure drop and mass-transfer characteristics

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Key words: Mass-transfer characteristics, Hydrodynamic performance, MellapakPlus packing

Structured packings such as MellapakPlus 252.Y belong to a modern generation of high-capacity column internals intended to provide effective gas-liquid contacting while avoiding hydraulic constraints. Thanks to their optimized corrugated-sheet architecture and inherently low pressure drop, MellapakPlus packings are commonly implemented in absorption, distillation, and stripping, where both high throughput and strong mass-transfer performance are required. The 252.Y configuration offers a well-balanced combination of specific surface area, capacity, and operational versatility, making it attractive for applications targeting high separation efficiency at reduced energy demand. Although MellapakPlus packings are widely used in industry, high-quality experimental hydrodynamic and mass-transfer data remain valuable for the validation of predictive tools and for improving design correlations. This work contributes by delivering a detailed experimental evaluation of the hydraulic and mass-transfer characteristics of MellapakPlus 252.Y under controlled absorption conditions.

Hydraulic performance was quantified by pressure-drop measurements in an air-water system over a broad range of gas and liquid loads. Mass-transfer properties were determined using three established reference systems: oxygen desorption from water for estimating the liquid-side volumetric mass-transfer coefficient ($k_L a$), chemisorption of SO_2 into aqueous NaOH to obtain the gas-side volumetric mass-transfer coefficient ($k_G a$), and chemisorption of CO_2 into aqueous NaOH for determining the effective interfacial area (a). To remove the influence of inlet and outlet regions, all mass-transfer parameters were evaluated using the subtraction method.

Experiments were performed in an atmospheric column with an internal diameter of 0.3 m and with packed-bed heights varied from 0.42 m to 1.3 m. The resulting dataset served to identify the hydraulic parameters (C_S, C_{Fl}, and $C_{P,0}$) and the mass-transfer parameters (C_L and C_V) of the Billet and Schultes (1999) model. The derived parameter set provides a consistent description of MellapakPlus 252.Y performance and supports reliable design and scale-up of absorption equipment employing this structured packing.

Fabrication of PDMS Membranes with Hierarchical Tapered Pores for Advanced Organ-on-a-Chip Applications

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Key words: Maskless lithography, Hierarchical microstructures, Microperforated membrane, Organ-on-a-chip

Elastic porous membranes are essential components of mechanically active organ-on-a-chip (OOC) and microphysiological system platforms, where they serve as critical tissue-tissue or tissue-environment interfaces allowing nutrient exchange, stretching, and optical clarity. Despite their importance, conventional fabrication methods often suffer from low reproducibility due to the formation of residual polymer films, which can compromise pore connectivity and device integrity. To address these challenges, this work explores fabrication strategies suitable for polydimethylsiloxane (PDMS) membranes featuring hierarchical tapered pores.

The methodology utilizes multilayer SU-8 epoxy photoresist masters consisting of hierarchical cylindrical micropillars. By gradually stacking arrays of cylinders of decreasing diameters, a 3D template is created for the casting of negative replicas, i.e., PDMS membranes with well-defined, tapered through-holes. The subsequent formation of PDMS membranes can be performed in several ways, and this work aims to identify the optimal procedure to achieve high yields and membrane quality, as well as true spatial dimensions and pore passability.

The resulting hierarchical geometry is intended to offer unique advantages for biomimetic applications. The tapered pores, combined with surface hydrophobization, are expected to exploit Laplace pressure to prevent liquid flow between air and liquid compartments, maintaining a stable air-liquid interface in lung-on-a-chip models. Furthermore, the functional performance of these membranes will be validated through size-selective filtration experiments using polystyrene beads of two distinct sizes – below and above the pore diameter – to demonstrate the potential for precise particle capture and cell separation. This research aims to provide a versatile platform for developing high-fidelity microphysiological systems with highly customizable transport properties.

Impact of counter-ion properties on ion-exchange membrane behavior

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Key words: electrodialysis, ion-exchange membranes, electroconvection, gravitational convection

Electromembrane separation processes, such as electrodialysis (ED) and electrodeionization (EDI), form a group of industrially essential separation techniques envisioned to play a significant role in achieving a fully circular economy. Their utilization is frequently associated with green, recyclable, environmentally friendly, zero-liquid discharge, and sustainable technologies. Electrodialysis, primarily designed for the separation of small ions from treated solutions, finds versatile applications ranging from water desalination and wastewater treatment to the processing of biologically relevant samples.

The typical ED stack consists of aligned ion-exchange membranes (IEMs) that enable selective ion transport under an applied electric field. The standard membrane arrangement involves a regular alternation of cation-exchange (CEM) and anion-exchange membranes (AEM), resulting in the formation of two output streams: a diluate and a concentrate.

A deeper understanding of the transport phenomena governing these processes is essential for their further optimization. In particular, electroconvection in the vicinity of ion-exchange membranes plays a crucial role, as it significantly influences mass transfer and overall system performance.

To investigate these effects, a custom-designed experimental setup was developed, allowing the implementation of a small membrane sample into an observation cell. The system is equipped with a microscope and a high-resolution camera, enabling direct visualization of the region near the membrane surface. Convective flow is monitored using tracer particles, and the velocity field is evaluated by means of Particle Image Velocimetry (PIV).

Although electrodialysis is commonly applied for seawater desalination, real saline systems contain, in addition to NaCl, a variety of other ionic species. Therefore, this study focuses on the influence of selected ions, namely F^-, Cl^-, Br^-, I^-, and SO_4^{2-}, on the intensity of electroconvection near the membrane, with particular emphasis on the effect of their concentration.

INVESTIGATION OF MEMBRANE DISTILLATION FOR THE RECOVERY OF VALUABLE PRODUCTS

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Key words: membrane distillation, membrane crystallization, lithium carbonate, hollow-fiber membrane module

Membrane distillation is a thermally driven membrane separation process based on the transport of water vapour through a porous hydrophobic membrane. Due to its ability to treat highly concentrated solutions at relatively low operating temperatures, membrane distillation represents a promising alternative for wastewater treatment, desalination and recovery of valuable compounds from liquid streams. This work is focused on the investigation of the possibilities of using direct contact membrane distillation for concentrating salt solutions and recovering valuable products, focusing on lithium carbonate crystallization. A laboratory-scale experimental apparatus with a hollow-fiber polypropylene membrane module was designed and operated in a counter-current arrangement. The study involved the construction using a 3D printer and subsequent testing of several membrane modules differing in design parameters such as module length, diameter and packing density. The influence of selected operating parameters, including retentate and permeate temperature, flow rate and initial salt concentration, on the transmembrane flux was experimentally investigated. In addition, a mathematical model describing heat and mass transfer in the membrane module was developed and compared with experimental data. The final part of the study examined the possibility of lithium carbonate crystallization directly in the retentate tank during membrane distillation, focusing on the effect of water removal rate on the quality of produced crystals. The work demonstrates the potential of membrane distillation as a hybrid separation and concentration process suitable for the recovery of valuable substances from concentrated aqueous streams.

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Metallized membranes for membrane distillation

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Key words: membrane distillation, polymer membrane, magnetron sputtering, metal coating

Abstract

Porous polypropylene capillary membranes were coated with nanoscale metallic layers (Au, Ag, and Cr) using magnetron sputtering and applied in membrane distillation (MD). The metallized membranes were assembled into submerged modules and their performance was experimentally evaluated. In submerged MD, heat and mass transfer are mainly controlled by a macroscopic boundary layer surrounding the membrane surface, which determines the overall transport resistance. In addition, a local near-wall boundary layer exists at the surface of individual membrane capillaries. The nanoscale metallic surface features introduced in this study primarily affect this near-wall region, enhancing thermal energy delivery to the evaporation interface while leaving the macroscopic hydrodynamics of the submerged module unchanged (Fig. 1). As a result, a moderate increase in permeate flux, reaching 20–30%, was achieved for the metal-coated membranes compared to unmodified ones, demonstrating the potential of controlled surface metallization for improving membrane distillation performance.

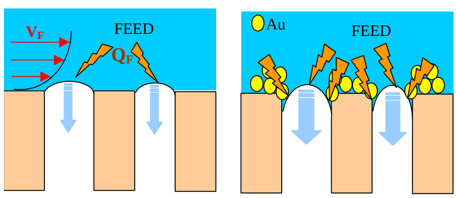

Fig. 1. Schematic model illustrating how metal deposition alters the meniscus shape and enhances heat transfer to the evaporation surface.

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Purification of succinic acid from fermentation medium using membrane separation

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Key words: succinic acid; trioctylamine; membrane module; competitive extraction; pertraction.

Succinic acid (SA) represents a key raw material for the production of biodegradable polymers and pharmaceuticals. Its biotechnological production via fermentation is a sustainable alternative to petrochemical processes. However, it faces technological barriers during product purification. In the solution, the target acid coexists with by-products such as formic acids (FA) and acetic acids (AA), making product isolation the most economically demanding part of the entire production cycle.

This work focuses on the systematic study of the equilibrium and kinetic characteristics of the reactive extraction and transport of these organic acids using the extractant trioctylamine (TOA) in a 1-octanol medium. Primary attention was devoted to the measurement of equilibria in single-component systems, confirming a strong dependence of extraction yield on the pH of the aqueous phase. The highest efficiency was achieved in the acidic region (pH 2–4), corresponding to the predominant undissociated form of the acids, providing a fundamental quantitative basis for understanding the acid-carrier interactions.

The core of the research involves the kinetics of single-component pertraction performed via capillary membrane module, where the time-dependent transport of each individual acid across a liquid membrane immobilized in the pores was systematically monitored. The measured kinetic curves of concentration changes in the feed and stripping phase provide essential data on mass transfer rates, diffusion and transport properties, and the intrinsic selectivity of the membrane system for each component. The obtained experimental data from these equilibrium and single-component kinetic measurements serve as the critical foundation for the formulation and validation of a mathematical model used to precisely predict system behavior and optimize the parameters of the separation process.

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Separation and Purification of Rapeseed Polyphenols

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Key words: rapeseed meal, polyphenols, adsorption

Polyphenols are valuable natural compounds with **increasing demand in food and cosmetics** due to their **natural bioactive** properties. Rapeseed meal (RSM), a major agri-industrial by-product of rapeseed processing, represents an abundant and underutilized source of phenolic compounds. Analysis of rapeseed meal produced within Envien Group showed that the total concentration of phenolic compounds was approximately 400 mg/kg, dominated by **sinapic acid**. This contribution focuses on the valorization of rapeseed meal through the development of efficient separation and purification technologies for polyphenol recovery, in line with sustainability and circular economy principles.
Our work investigates **rapeseed meal-derived feedstocks** as source of polyphenols. Sinapic acid accounts for more than 85 % of all quantified phenolic acids in rapeseed meal, with minor contributions from protocatechuic, 4-hydroxybenzoic, and ferulic acids (ca. 10 % combined). The proposed pilot process integrates solvent extraction, membrane filtration for protein-containing streams, and adsorption on polymeric resins followed by ethanol desorption. Systematic adsorbent screening, and equilibrium and kinetic studies were performed to support process optimization and scalability. For powder production, vacuum drying as well as lyophilization were tested. The examined polyphenol applications cover skincare cosmetics and natural preservatives in food.
Pilot-scale experiments confirm the feasibility of scaling up polyphenol recovery while maintaining compatibility with existing rapeseed meal and protein isolate processing lines. Overall, the developed process enables the production of high-value rapeseed-derived polyphenol extracts and supports the **integration of circular bioeconomy** and creation of new supply chains with focus on material sustainability.

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Separation of Acidic Gases from Humid Flue Gas Using Advanced Membrane

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

Combustion technologies constitute a major source of industrial emissions. In addition to solid by-products, combustion processes generate a wide range of compounds that are released in the gaseous phase. Various flue gas treatment methods are currently implemented to ensure compliance with emission limits prior to atmospheric discharge. However, these technologies are increasingly approaching their intrinsic limits in terms of separation efficiency.
The objective of this study is to investigate the performance of novel membrane materials using a custom-designed experimental apparatus for the separation of gaseous mixtures under humid conditions representative of real operating environments. The automated testing system is equipped with a membrane module featuring a variable effective membrane area, water vapor saturators, and humidity sensors installed on all process streams, enabling rapid and precise adjustment of experimental conditions. Furthermore, the system incorporates a gas analyzer capable of quantifying acidic components, such as CO_2 and SO_2, within complex gas mixtures.
Within this work, the purification of feed gas to levels compliant with European Commission legislative requirements is demonstrated using a thin-film composite membrane with a polyamide and polyethyleneimine selective layer under humid conditions. In addition, other polymeric membrane materials, including those based on ionic liquids and polymers of intrinsic microporosity, were evaluated using single gases and their mixtures across a range of feed pressures. Their separation performance, expressed in terms of permeability, selectivity, and stage-cut, is systematically analyzed.

The effect of unwanted H+ permeation through anion exchange membranes on the electrodialysis process with bipolar membranes

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Key words: electrodialysis; bipolar membrane; proton blocking membrane

Electrodialysis with bipolar membranes (EDBM) is a unique electromembrane process capable of generating acids and bases from solutions of their salts. If the performance of this process is to be controlled, the properties of the membranes used play a key role. Experimental comparison of different membrane combinations has shown that, in order to achieve high salt flux, low specific energy consumption, and high product concentrations, it is desirable to use anion exchange membranes (AEM) and cation exchange membranes (CEM) with the ability to block H^+ and OH^- ions, respectively [1]. The aim of this study was to experimentally demonstrate the significant impact of undesirable H^+ ion transfer through AEM on the EDBM process and to propose and verify possible methods for its optimization. A set of laboratory EDBM tests was conducted, clearly showing that the transport of H^+ ions into the diluate from the acid loop increases with increasing acid concentration. This phenomenon significantly reduces current efficiency, lowers the concentration of both products, and may even lead to the practical cessation of diluate desalination. Based on the data obtained, three approaches were proposed to mitigate these negative effects:
(1) operating the process in batch mode, allowing the acid concentration to increase gradually over time so that the associated adverse effects appear as late as possible;
(2) continuous neutralization of the acidic diluate, for example using the produced alkali, particularly in applications, where achieving a certain degree of diluate desalination is essential;
(3) limiting the maximum concentration of the produced acid by dilution with water, in cases where it is more important to reach the desired base concentration or to desalinate the diluate.

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[1] Slovák, F., Kotala, T., & Václavíková, N. (2025). Comparison of different combinations of heterogeneous and homogeneous bipolar and ion exchange membranes in lab-scale electrodialysis stack. *Chemical Engineering Communications*, 212(9), 1332–1340.

Posters: Reaction engineering and catalysis

A comparative study of various Pr(La)SrBaCeCo(Ni)Ox compounds for total oxidation of ethanol

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Key words: volatile organic compounds, catalytic oxidation, peroskites

This work presents a comparative study of several Co-based perovskite catalysts with varying compositions and structures for the oxidation of ethanol, representing VOCs. Perovskite oxides of the ABO_3 type are highly efficient catalysts for the oxidation of volatile organic compounds (VOCs) because they offer high thermal stability and the possibility to tune their composition. Two types of Pr(La), Ba, Ce, Sr, Co(Ni) mixed oxides with various molar ratios were prepared by the Pechiney method (sintering of a mixture of nitrates, citric acid, and ethylene glycol at 950 °C) and coprecipitation (metal nitrates were precipitated with an alkali solution of Na_2CO_3 and NaOH, and the product calcined at 700 °C).
Powder XRD revealed the formation of various kinds of perovskites ($SrCoO_{2.8}$, $Pr_{1.5}Sr_{0.5}NiO_4$, $BaNiO_3$, $BaCeO_3$, $La_{1.16}Sr_{0.77}NiO_{3.94}$), along with oxides and carbonates, in the sintered catalyst. In contrast, $Pr_{0.33}Sr_{0.67}(CoO_{2.7})$ perovskite, along with various oxides and carbonates, was found in the precipitated catalysts. The surface area of the sintered catalysts was about 2 m^2g^{-1}, while that of the precipitated catalysts was about 14 m^2g^{-1}. XPS measurements showed that the surface cobalt concentrations in both types of catalysts were roughly half of that of the bulk composition. The most active catalysts achieved complete ethanol oxidation below 200 °C and showed high selectivity toward CO_2. Catalytic activity was higher for precipitated catalysts. Their T_{50} values were almost half that observed for sintered catalysts. The low activity is most likely due to the small surface area. Typical for the investigated perovskite catalysts is a very low concentration of CO as a reaction by-product. These findings highlight the potential of tailored perovskite catalysts for efficient VOC abatement.

Evaluation of the self-cleaning efficiency of g-C_3N_4 surfaces as a function of temperature and humidity

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This work focuses on the study of self-cleaning properties of surfaces modified with thermally exfoliated graphitic carbon nitride (g-C_3N_4), which represents a promising photocatalytic material active in the visible region of the spectrum. The prepared material was applied to model substrates, and its self-cleaning efficiency was evaluated according to the UNI 11259:2008 standard, based on the degradation of the organic dye Rhodamine B. Experimental measurements were carried out in a climate chamber under simulated daylight illumination. The influence of various combinations of temperature and relative humidity on the rate of photocatalytic dye degradation, and thus on the self-cleaning efficiency, was systematically investigated with the aim of approximating real outdoor conditions.

The results show that both, temperature and relative humidity significantly affect the photocatalytic activity of the prepared surfaces. Conditions leading to optimized self-cleaning performance were identified, as well as regimes where the efficiency is limited. These findings contribute to a better understanding of the behavior of g-C_3N_4-based materials under realistic application conditions and may serve as a basis for their practical use in outdoor self-cleaning coatings. The presented work thus provides important insights into the influence of environmental factors on the performance of photocatalytic surfaces and contributes to their more efficient design for practical applications.

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Toward Green NH_3 Electrosynthesis: Nanocatalysts, 3D-Printed Electrodes, and Electrolyzer Design

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Key words: green ammonia, electrosynthesis, MOF-derived nanomaterials, 3D-printed electrodes, electrolyzer design

Ammonia is a key industrial chemical for fertilizer production and is increasingly considered as an energy carrier and hydrogen storage medium. Its current manufacture relies almost exclusively on the Haber–Bosch process, which is highly energy-intensive and dependent on fossil-derived hydrogen. Electrochemical ammonia synthesis is therefore attracting interest as a more sustainable alternative because it can, in principle, operate under mild conditions, use renewable electricity, and be implemented in modular systems. However, practical application remains limited by challenges in selectivity, Faradaic efficiency, productivity, and control of the local reaction environment. Here, we outline a multiscale route toward green NH_3 electrosynthesis based on the combined development of nanocatalysts, 3D-printed electrodes, and electrolyzer design. At the nano level, hierarchically structured metal-organic framework (MOF)-derived nanomaterials represent a promising platform for advanced electrocatalytic materials. Rapid synthesis routes, such as microwave-assisted processing, combined with controlled post-treatment, for example by laser irradiation, enable composites with tunable active surfaces, high accessible surface area, abundant active sites, and coupled micro-/mesoporosity. These features may improve NH_3 selectivity, increase Faradaic efficiency, and provide better control over competing interfacial pathways. At the meso level, 3D-printed triply periodic minimal surface (TPMS) electrodes offer a systematic route to tune porosity, flow-channel dimensions, and the balance between surface area and mass transport. In such structures, geometry, roughness, wettability, and electrolyte convection act as active design variables that influence interfacial transport, gas-bubble dynamics, and overall electrochemical response. At the macro level, the concept evolves from a lab-scale stationary H-cell to flow-cell configurations and, ultimately, toward integrated electrolyzer design. Across all stages, 3D printing enables rapid fabrication and iteration of reactor components, while computational fluid dynamics (CFD) modelling supports optimization of flow distribution, transport behavior, and overall design performance. Together, these elements define a stepwise engineering pathway toward more stable, efficient, and scalable NH_3 electrosynthesis systems.

Posters: Material engineering and design

Advanced SiO_2-based adsorbent for CO_2 capture

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Key words: CO_2 capture, periodic mesoporous organosilica, amine functionalization, CO_2/N_2 selectivity

The increasing need to reduce carbon dioxide emissions has intensified research into efficient solid adsorbents for post-combustion CO_2 capture. Intensive research has therefore been devoted to advanced adsorbents such as zeolites, porous carbons, metal–organic frameworks (MOFs), and metal oxides. In recent years, amine-functionalized mesoporous materials have attracted particular attention because amino groups exhibit strong affinity toward CO_2. These materials often combine high adsorption capacity, rapid kinetics, easy regeneration, and good cyclic stability. Mesoporous silica is especially attractive, and its CO_2 capture performance can be significantly enhanced by grafting amine-containing compounds onto the surface [1,2].

This study investigated the CO_2 adsorption properties of amine-functionalized mesoporous silica and organosilica materials. Ordered mesoporous supports were synthesized and subsequently modified with an amine-containing silane coupling agent. Textural characterization confirmed the preservation of mesostructured porosity, high specific surface area, and narrow pore size distribution after functionalization. The modified materials showed substantially higher CO_2 adsorption capacities than the original samples, particularly under ambient conditions. Additionally, amine grafting significantly improved CO_2/N_2 selectivity, indicating enhanced separation performance. Overall, these results demonstrate that amine-functionalized mesoporous silicas are promising candidates for efficient and selective CO_2 capture applications.

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Comparison of the sorption properties of starch from Horse chestnut (Castanea sativa Mill.) and London plane tree (Platanus acerifolia) fruits

Abstract: Plantain, commonly referred to as a cooking banana, and sweet chestnut, known as marron, are tree fruits that are commonly found only in selected regions of the world. The fruits of both plants grow on trees, which undoubtedly constitutes a shared characteristic. Moreover, both plantain and sweet chestnut are rich sources of dietary fiber, vitamin B6, vitamin C, and potassium. Therefore, it is worthwhile to seek as many applications as possible for these valuable raw materials. Increasing attention has recently been paid to gluten-free diets in the context of celiac disease. Both plantain and sweet chestnut are processed into powdered forms with a high starch content. It is possible that these gluten-free powders exhibit properties similar to those of gluten-containing flours and may become useful in everyday culinary practice for individuals with celiac disease. The aim of the present study was to compare the hygroscopic properties of two high-starch powders obtained from the fruits of sweet chestnut (Castanea sativa Mill.) and London plane tree (Platanus acerifolia). The comparison of these properties was carried out on the basis of sorption isotherm parameters identified using the Brunauer–Emmett–Teller (BET) and Guggenheim–Anderson–de Boer (GAB) models. The empirical data forming the basis for the application of the BET and GAB transformations were obtained using the static desiccator method. Water content was determined in accordance with the Polish standard PN-EN ISO 712:2012 using an SLW 75 SMART laboratory dryer. Water activity was measured using an AquaLab 4TE device (Decagon Devices, Inc., Pullman, WA, USA). The size, shape, and number of particles in the tested powders were characterized using a Morphologi G3 automatic particle analyzer (Malvern Instruments). The obtained results indicate that the tested powders differed in their initial state, both in terms of the size and shape of the particles composing them, as well as in terms of their initial water content and water activity. Particles of the plane tree powder bound water more strongly than particles of the sweet chestnut powder. The course of the sorption isotherms also indicated that these powders differed in terms of hygroscopicity. The identified isotherm parameters demonstrated that the interaction between the particles of both powders and water molecules was physical in nature. The monolayer capacity of plane tree powder particles was 1.6 to 2.1 times greater than that of sweet chestnut powder, which confirms its higher hygroscopicity. Analysis of the results in terms of size and shape parameters showed that particles of the plane tree powder were larger and more massive than those of the sweet chestnut powder. Both tested powders were characterized by a shape markedly deviating from circularity, while particles of the plane tree powder were additionally distinguished by lower convexity. This observation, indicating a greater development of the particle surface in the plane tree powder, may be associated with its higher monolayer capacity and greater ability to bind water, which in turn leads to a reduction in water activity. The findings of this study provide new information relevant to the management of the production process, as well as to the safety and stability of these powders.

Encapsulation strategies for studying soil bacterial interactions

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Key words: microbial encapsulation, quorum sensing, controlled release

Microbial interactions in soil, including those mediated by quorum sensing, are strongly influenced by spatial organization and cell-to-cell communication. However, investigating these processes under controlled conditions remains challenging, particularly in systems involving bacteria–fungi interactions. This work addresses this limitation by employing microbial encapsulation as a strategy for controlled spatial organization of soil bacteria using alginate beads. Model Gram-negative and Gram-positive soil bacteria were immobilized in alginate matrices, with the addition of polyvinyl alcohol (PVA) to tune mechanical stability and bacterial release kinetics, while chitosan was applied as a surface coating to further modulate matrix permeability. Encapsulation performance was assessed by determining viable cell counts (CFU) within the encapsulated matrix and quantifying bacterial release from the beads over time. The influence of formulation parameters, including PVA content and chitosan coating, on bacterial retention and stability was systematically evaluated. Preliminary results show that viable cell populations are maintained within alginate beads, while increasing PVA content reduces bacterial release. Initial experiments with chitosan-coated beads indicate further potential for limiting release through surface modification of the matrix.

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Preparation of Microstructures and Their Integration into a Microfluidic Platform for Biofilm Assays

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Keywords: microstructures, biofilm, lithography, microfluidic platform

Bacterial biofilms represent complex structures formed by bacteria. Within this specific arrangement, cells communicate much more effectively and, most importantly, they exhibit significantly higher resistance to antimicrobial agents compared to their planktonic form. For this reason, it is essential to explore biofilm formation and its resistance to environmental conditions such as shear rate, as well as the antimicrobial effect of different agents. It is well established that the topography of the surface represents a key factor influencing bacterial behavior, as it can fundamentally modify processes such as cellular adhesion or bacterial morphology.

This work focuses on the design and fabrication of microstructured surfaces using laser lithography. Specifically, the research addresses the creation of two-layer structures. These structures primarily serve as a master mold for subsequent surface replication via soft lithography, which represents a crucial step toward the successful fabrication and assembly of a functional microfluidic platform.

A substantial part of the entire research is dedicated to the detailed optimization of the fabrication process parameters of microstructures. These parameters, such as exposure dose or focus correction, play a critical role, as they directly influence the final morphology, dimensional accuracy and overall quality of the prepared microstructures, which are essential for ensuring the reliability and reproducibility of future experiments.

In the initial phase, the fabricated microstructured surfaces will be subjected to testing under static conditions to evaluate their primary effect on bacterial cell behavior. The main objective of this step is to determine whether the specific surface topography inhibits the formation of microcolonies. Once these fundamental interactions between bacteria and the surface are characterized, the experimental design will advance to the dynamic phase. The microfluidic platform will be connected to syringe pumps and will be operated in a continuous flow regime. This will simulate physiological and environmental conditions more accurately, including the effect of hydrodynamic shear stress. In this setup, the dynamics of biofilm development will be monitored and evaluated in detail, with the results from the structured chip being compared against reference data from a control chip with a smooth, unstructured surface.

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Self-Assembled Pectin-based Nano/Microcapsules in Fruit Pastilles: A Strategy for Clean-Label Nutraceuticals with Improved Stability and Bioactivity

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Key words: clean label, nanoencapsulation, pectin self-assembly, functional food, propolis, sea buckthorn oil, antibacterial activity

The growing demand for "clean label" functional foods necessitates the development of products that not only promote health but also possess high sensory quality. Fruit-based products provide an excellent matrix for enrichment with bioactive ingredients, appealing to a broad range of consumers. The aim of this study was to develop an innovative, simple, and eco-friendly technology for producing fully natural, health-promoting fruit pastilles containing nano/microcapsules with bioactive ingredients (propolis, sea buckthorn oil). A novel encapsulation and production method was established, consisting of: (a) mechanical homogenization of fruit pulp (plums, apples) to release and disperse endogenous pectin; (b) formation of a nanoemulsion of bioactive ingredients using ultrasonic homogenization; (c) combining both fractions via ultrasound treatment, inducing the self-assembly of pectin into shells encapsulating the nanoemulsion droplets; and (d) forming and drying the final product. This technique yielded stable nano/microcapsules with a diameter of 0.1–5 µm and a pectin shell thickness of 5–100 nm, fully integrated within the fruit matrix. Electron microscopy confirmed the proper morphology of the capsules. The capsule-enriched products exhibited more favorable textural properties (reduced hardness) compared to control samples. A key achievement was significantly improved stability; after 6 months of storage, the product retained its organoleptic properties, whereas non-encapsulated samples underwent degradation (oil rancidity). Furthermore, the products demonstrated significant local antibacterial activity against upper respiratory tract pathogens, such as *Staphylococcus aureus*, confirmed by distinct growth inhibition zones. The obtained products can serve as natural nutraceuticals with extended shelf life and potential supportive effects in throat infections, setting a new direction in the design of clean-label, smart foods and dietary supplements.

Surface Modification of Waste-Derived Hematite Pigments with Nano-Oxides for Enhanced Colloidal and Optical Properties

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Key words: hematite pigments, waste valorization, surface modification, nano-oxides, colloidal stability

Abstract

The development of high-performance pigments from industrial by products is a key step toward a circular economy in the coatings industry. This study investigates the synthesis of hematite (α-Fe_2O_3) pigments from waste-derived iron(II) sulfate using a microwave-assisted method and their subsequent surface modification with TiO_2, SiO_2, and Al_2O_3 nanoparticles. The base pigments, synthesized at varying pH levels (8, 10, and 12), exhibited distinct morphologies, including well-defined cubic and highly faceted structures. To prevent secondary agglomeration and tailor surface reactivity, a mechanical coating process via milling was employed.

Results from SEM and DLS analyses confirm the successful deposition of nano-additives, leading to a 2.5 to 11-fold reduction in mean particle size compared to the base pigments. While the modifications significantly improved dispersibility and reduced oil absorption (particularly with 10 wt% Al_2O_3), the intrinsic red color of the hematite remained visually consistent, with ΔE values typically remaining below the threshold of perceivable change. Furthermore, electrokinetic studies revealed that nano-oxide selection allows for precise tuning of the isoelectric point (IEP), ranging from strongly acidic (IEP $\approx$ 2.6 for SiO_2) to basic (IEP > 9 for Al_2O_3). These findings demonstrate an efficient route to producing sustainable, functionalized pigments with tunable surface properties suitable for advanced industrial coatings.

Posters: Pharmaceutical engineering and processes

Spray-dried allicin/β-cyclodextrin inclusion complexes for antimicrobial applications

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Key words: allicin, antimicrobial resistance, spray drying, inclusion complexation, β-cyclodextrin

Antimicrobial resistance is a rapidly growing threat to global medicine, primarily driven by the misuse and environmental accumulation of conventional antibiotics. Prolonged exposure of bacteria to subinhibitory concentrations facilitates the rapid development of resistance mechanisms. An innovative strategy to combat this challenge involves utilizing highly reactive antimicrobial agents with a short environmental half-life, thereby minimizing the evolutionary window for bacteria to develop resistance. A promising candidate is allicin, a natural broad-spectrum antimicrobial compound derived from garlic (*Allium sativum*). Allicin, natively not present in intact tissue, is synthesized upon cellular rupture when the precursor alliin and the enzyme alliinase, normally segregated in different cellular compartments, interact as a defense mechanism responding to immediate cell damage. However, allicin's inherent chemical instability poses a significant hurdle to its practical therapeutic application.

In light of these challenges, the primary objective of this research is to stabilize the allicin molecule via inclusion complexation with β-cyclodextrin (β-CD), a cyclic oligosaccharide whose hydrophobic cavity accommodates and shields the guest molecule from thermal and photochemical degradation. To isolate these complexes in a stable solid form, spray drying was employed, efficiently converting the liquid allicin/β-CD feed into a fine, dry powder. Crucially, although spray drying of aqueous solutions utilizes higher inlet gas temperatures, the rapid evaporative cooling effect ensures that the droplets and the resulting powder are mostly exposed to the significantly lower wet-bulb temperature. This thermodynamic mechanism makes the process highly suitable for preserving heat-sensitive compounds such as allicin.

The powder composition was optimized and subsequently evaluated for *in vitro* antimicrobial efficacy, along with comprehensive testing to assess its long-term stability under various storage conditions. Also, the performance of the allicin/β-CD powders was compared with previously developed spray-dried inhalable carriers co-encapsulating allicin precursors.

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