



Chemical Engineering Day at UCTM

2024

Ден на Инженерната ХИМИЯ В ХТМУ



University of chemical technology and metallurgy

Програма на "Ден на Инженерната Химия в ХТМУ", 29 ноември 2024

1. Пленарна сесия от 10:00 до 12:00 часа в зала „Асен Златаров“ на ХТМУ

10:00 - 10:15 - Откриване на събитието от проф. Сеня Терзиева-Желязкова, Ректор на ХТМУ, както и представяне на катедра „Инженерна Химия“ към ХТМУ от ръководителя й доц. Чавдар Чилев

10:15 - 10:45 - Научен доклад от гост професор, Проф. Gyorgy Szekely, "Towards a sustainable and energy-efficient future with membranes"

10:45 - 11:00 - Фирмен доклад на Алмагест ЕООД - Производство на етанол от зърнени култури

11:00 - 11:15 - Фирмен доклад на B2N ООД - Пионер в 3D индустрията на Балканите

11:15 - 11:30 - Фирмен доклад на Релина ЕООД - Производство на food и pharma продукти

11:30 - 11:45 - Фирмен доклад на Технофос АД - Иновации във фосфатните технологии

11:45 - 12:00 - Фирмен доклад на Германо-Българската индустриално-търговска камара (ГБИТК) - Първият и основен партньор на представителите на германската икономика в България

2. Постерна сесия „Академия и индустрия“ и фирмено изложение от 12:00 до 15:00 в БиЦ на ХТМУ

12:00 - 13:00 - Провеждане на постерната сесия, съпроводено с коктейл и get-together

12:00 - 15:00 - Паралелно фирмено изложение с обособени фирмени щандове и демонстрации.

Участващи фирми с щанд ще бъдат: B2N ООД, Релина ЕООД, Елаците Мед АД, Региоком Европейско Дружество България, Химкомплект-Инженеринг АД, Аурубис България АД, Лиебхер-Хаусгерете Марица ЕООД.

Program of the "Chemical Engineering Day at UCTM", November 29, 2024

1. Plenary session from 10:00 to 11:45 in the "Assen Zlatarov" hall of the University of Chemical Technology and Metallurgy - Sofia

10:00 - 10:15 - Opening of the event by Senya Terzieva-Zhelyazkova, Rector of UCTM, and presentation of the Department of "Chemical Engineering" at UCTM by its Head, Assoc. Prof. Chavdar Chilev

10:15 - 10:45 - Scientific report by guest professor. Prof. Gyorgy Szekely, "Towards a sustainable and energy - efficient future with membranes"

10:45 - 11:00 - Company report from Almagest - Production of bioethanol

11:00 - 11:15 - Corporate Presentation by B2N - Pioneer in the 3D industry in the Balkans

11:15 - 11:30 - Corporate Presentation by Relina - Production of food and pharma products

11:30 - 11:45 - Corporate Presentation by Technophos - Innovations in phosphate technologies

11:45 - 12:00 - Corporate Presentation by The German-Bulgarian Chamber of Industry and Commerce (АНК Bulgaria) – The first and key partner for representatives of german business in bulgaria

2. Poster session "Academy and Industry" and company exhibition from 12:00 to 15:00 in the Library and Information Center (BIC) of the University of Chemical Technology and Metallurgy – Sofia

12:00 - 13:00 - Poster session, accompanied by a cocktail and discussions

12:00 - 15:00 - Parallel Corporate Exhibition with dedicated company stands and live demonstrations.

Participating companies with stands: B2N, Relina, Ellatzite Med, Regiocom Bulgaria, Chimcomplex- Engineering, Aurubis Bulgaria, Liebherr-Hausgeräte Marica

Scientific committee

Prof. Eng. Senya Terzieva-Zhelyazkova, PhD

Assoc. Prof. Dimitar Peshev, PhD

Assoc. Prof. Ivaylo Hinkov, PhD

Assoc. Prof. Chavdar Chilev, PhD

Oral scientific presentation

Towards a sustainable and energy-efficient future with membranes

Gyorgy Szekely

Advanced Membranes and Porous Materials Center, Chemical Engineering Program,
Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology
(KAUST), Saudi Arabia

Separations are extensively used across numerous industrial sectors. Membranes offer a sustainable and energy-efficient way for separations. These membranes must be stable under harsh conditions, have high selectivity and permeance. There is a need to develop sustainable membrane materials and processes. Biomass-based building blocks can replace fossil-based separation materials and reduce waste generation. The exploration of various green sources to fabricate solvent-resistant nanofiltration membranes will be presented. The design of sustainable thin-film composite membranes via interfacial polymerization of green building blocks will be discussed. The use of these green membrane materials in energy-efficient separation processes will be introduced. We established the OSN Database, an open-access platform to share data and models. The recent progress in numerical optimization models has been significantly boosted by the availability of large datasets and the rapid advancements in computational power, driving major enhancements in process and material design. These developments have facilitated the optimization of hyperdimensional spaces through machine learning and deep learning where analytical solutions are not feasible. Case studies exploiting machine learning models to design better separation processes will be discussed. Our predictive models are freely accessible on the OSN Database, fostering a collaborative and inclusive approach to advance sustainable separations.

List of Poster Presentations

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- Poster 4: Rapeseed Protein Extraction for Aquaculture Nutrition
- Poster 5: Sulfuric acid autoclave treatment of zinc ferrite cake
- Poster 6: Application of NMR spectroscopy in alcoholic grape beverages
- Poster 7: Enhanced heating systems for fluidized bed reactors: innovations and applications
- Poster 8: Development of a measurement method for determining the drying kinetics of volatile water and alcohol components in solids
- Poster 9: 3D design and research of a continuously operating bioreactor with mechanical agitation and aeration
- Poster 10: Study of the mixing process of two immiscible liquids
- Poster 11: Optimization of the dispersion process in the production of industrial coatings
- Poster 12: Green solvent extraction and separation of 4f-ions with chelating ligands: mechanistic modelling
- Poster 13: A study on encapsulation of lavender oil essence in zeolite and bentonite-based matrices
- Poster 14: Development of multicomponent glasses for application as a glazing layer on dental zirconia
- Poster 15: Guerbet condensation of 1-butanol over zeolite catalysts
- Poster 16: Technology and installation for purification and neutralization of acid gases
- Poster 17: Academic English and German: Chemical and Biochemical Engineering
- Poster 18: An integrated novel approach to the sustainable recovery of bioactives from *Croton lechleri* twigs
- Poster 19: On the influence of Soxhlet operating conditions on extract yield of Cornelian cherry stones – a neglected waste
- Poster 20: Synthesis and characterization of heterocyclic hydrazones with biological application
- Poster 21: Modelling of the extraction kinetics of *Melissa officinalis*
- Poster 22: Testing of a conventional method for the analysis of gold from gold-bearing copper concentrates at "Ellatzite - Med" JSC
- Poster 23: Spontaneous deposition of Pd-Ag particles on carbon screen printed electrodes
- Poster 24: Water purification from 1,2-Dichloroethane and 1,2-Dibromoethane using some bacterial strains
- Poster 25: Acidic Lignocellulosic Hydrolysates: New achievements in their detoxification by liquid – liquid extraction with ionic liquids
- Poster 26: Partial dealcoholization of red wine Mavrud by nanofiltration
- Poster 27: Waste coffee grounds - millions of tons of waste or a source of valuable substrate for high value-added products?
- Poster 28: Multi-parameter optimization of polymer nanocomposites under combined loading

Poster 29: UV-assisted grafting as a tool for surface modification of polyethersulfone nanofiltration membranes

Poster 30: Green eco-friendly UV chemometric methods for simultaneously quantifying of four component anti-migraine drug formulation Paracofdal

Poster 31: Total antioxidant activity and total phenolic concentration in plant raw material

Poster 32: Biogas - an alternative to fossil fuels

Poster 33: Application of membrane filtration and spray drying technologies for the recovery of antioxidants from spent lavender

Poster 34: DNA fragmentation and apoptosis induction by polymer nanocarriers loaded with anticancer podophyllotoxin or juniper extracts

Poster 35: Evaluation of Heterogeneous Environmental Catalysts Using Temperature-Programmed Desorption, Reduction, and Oxidation – Methods and Applications

Poster Presentations

Poster 1:

Effect of Drying Methods on Protein Denaturation in Mealworm (*Tenebrio molitor*) Flour

Halime Idakiev¹, Danika Aleksandrova¹, Nicole Vorhauer-Huget²

¹University of Chemical Technology and Metallurgy Sofia, Bulgaria

²Otto-von-Guericke-University Magdeburg, Germany

The growing global demand for protein, fueled by rapid population growth, necessitates the development of sustainable production methods with minimal environmental impact. Mealworms (*Tenebrio molitor*) present a promising, eco-friendly protein source for both feed and food applications. In large-scale mealworm production, optimizing drying techniques is crucial for preserving product quality. This study explores the effects of freeze-drying and oven drying at 40 °C and 60 °C on protein denaturation in mealworms, using Differential Scanning Calorimetry (DSC) to evaluate protein integrity.

High-temperature oven drying results in darker coloration and a reduction in protein thermal stability, as well as lower residual moisture content. In contrast, freeze-drying preserves both color and protein integrity, although it retains higher moisture levels. Despite the longer processing times and higher energy consumption associated with freeze-drying, which may limit its industrial feasibility, it is more effective in maintaining native protein structures. Thermogram analysis reveals significantly higher endothermic peaks for freeze-dried samples, indicating greater energy absorption due to protein denaturation. The increased energy required for complete denaturation of freeze-dried samples suggests a better preservation of native protein structures.

Poster 2:

Mechanochemistry in Reuse of Spent Automotive Catalysts toward their Sustainable Recycling

A. Vasileva¹, K. Ivanov¹, D. Paneva¹, E. Encheva³, M. Shopska¹, I. Yakoumis², Z. Cherkezova-Zheleva¹

¹Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

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³Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

Spent automotive catalysts contain precious metals from the platinum group (PGMs) like platinum, palladium, and rhodium, which are essential for reducing harmful vehicle emissions. Although present in trace amounts, the annual demand for PGMs is high, making recycling crucial for conserving resources and reducing environmental impact.

Recycling methods include Regeneration, Direct Use, and Non-Direct Use, which help conserve PGMs, reduce costs, and minimize emissions by decreasing the need for new mining. The recycling process not only recovers PGMs but also reuses components like cordierite and rare earth elements, promoting sustainability.

Mechanochemical methods, which use mechanical energy to activate materials and initiate chemical reactions, offer an eco-friendly approach to PGM recovery. This study focuses on mechanochemical activation to enhance PGM accessibility on catalyst surfaces. Techniques such as XRD, XPS, SEM/EDS, and FTIR were used to analyze treated materials, confirming the presence of PGMs and improved catalytic sites.

Mechanochemical activation increased the catalytic efficiency of recycled catalysts, making them valuable for new catalyst synthesis. This approach aligns with green chemistry principles, reducing hazardous reagents and environmental impact, while improving the performance of multi-metallic PGMs in CO oxidation reactions.

Poster 3:

Characterization and Catalytic Behavior of Materials Prepared from Recycled Platinum in Spent Automotive Catalysts

K. Ivanov¹, A. Vasileva¹, Z. Cherkezova-Zheleva¹, I. Yakoumis², E. Encheva³, M. Shopska¹, I. Christova¹, D. Paneva¹, A.M. Moschovi²

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The catalytic recycling of platinum group metals (PGMs) from spent automotive catalysts (SACs) has become increasingly important due to the rising scarcity and high market prices of these metals. PGMs are essential in catalytic converters for reducing harmful vehicle emissions and are classified as critical raw materials due to their high demand and limited supply. Consequently, sustainable recycling technologies are being developed to reuse these metals in new catalysts.

In this study, PGMs recovered from end-of-life diesel oxidation catalysts (DOCs) were used to synthesize Cu-Pt-based catalysts supported on a CeO₂-ZrO₂ mixed oxide via the wet impregnation method. A single-step hydrometallurgical process was employed for efficient PGM extraction. The catalysts, designated as Sample A and Sample B, underwent different pretreatments: calcination for Sample A and hydrogen reduction followed by calcination in air for Sample B.

Characterization techniques, including X-ray diffraction (XRD), BET surface area analysis, and Fourier-transform infrared (FTIR) spectroscopy, revealed the structural and functional properties of the materials. BET analysis showed consistent surface area and porosity, while FTIR indicated the presence of active functional groups crucial for catalytic reactions. Sample B, pre-reduced before calcination, exhibited superior catalytic properties, suggesting optimized surface characteristics.

This research highlights the potential of SAC recycling for reclaiming PGMs and reusing them in catalytic applications, offering both environmental and economic benefits.

Poster 4:

Rapeseed Protein Extraction for Aquaculture Nutrition

Halime Idakiev, Vesselin Idakiev

University of Chemical Technology and Metallurgy Sofia, Bulgaria

Aquaculture is the fastest-growing animal food-producing sector, driven by increasing demand for fish as a primary source of protein for human consumption. However, the global supply of fishmeal, the main protein ingredient in fish diets, is insufficient to meet the demands of the expected growth in aquaculture. As a result, the industry's future depends on finding sustainable, high-quality alternatives for fish feed. Recent research has focused on replacing fishmeal with oilseed-based meals. One promising option is rapeseed meal, a by-product of rapeseed oil production, which offers a valuable protein source for use in aquafeed formulations.

To produce a rapeseed protein concentrate (RPC), small-scale pilot processing procedures were employed. The rapeseed meal for protein extraction was gently processed, followed by an aqueous extraction method to isolate the protein fractions. The resulting protein solution was purified and then dried. This rapeseed protein extraction process yields RPC with high nutritional value and minimal levels of antinutritional factors. Nutritionally, the produced RPC is comparable to fishmeal, with an amino acid profile that meets the amino acid requirements of fish.

The obtained RPC was used in experimental trials to replace fishmeal in the diets of rainbow trout, turbot, common carp, and wels catfish. The results of these feeding trials highlight the significant potential of RPC as a protein source in aquafeeds. The highest level of fishmeal replacement (up to 100%) was achieved in the rainbow trout trials. Based on these findings, RPC was identified as an excellent alternative to fishmeal, particularly in rainbow trout nutrition.

Poster 5:

Sulfuric acid autoclave treatment of zinc ferrite cake

Petar Iliev, Nadejda Kazakova, Iva Stoqnova, Miroslav Iliev, Nikola Angelov

University of Chemical Technology and Metallurgy Sofia, Bulgaria

The Bulgarian mining industry and its related metallurgy are modern industries, but the increased requirements of the EU regarding carbon-neutral technologies will lead to the replacement of the existing pyrometallurgical reduction technologies with new innovative hydrometallurgical ones.

In this regard, the mineral processing industry will have a serious impact on the environment not only due to the high consumption of energy, water and reagents, but also due to the large amounts of waste products generated after these industrial activities. These waste materials can be considered valuable newly generated man-made raw materials because they are obtained in large quantities as by-products of existing metallurgical activities and are a rich source of valuable metals. For example, in the production of 1 ton of zinc, 300 tons of zinc cakes are generated in the leaching of zinc calcine, which contain valuable non-ferrous and precious metals such as lead, silver, copper and indium.

The present work presents the results of laboratory experiments on sulfuric acid autoclave treatment of zinc ferrite cake with the aim of selective extracting zinc, copper and iron in solution and concentrating silver and lead in the undissolved residue.

Poster 6:

Application of NMR spectroscopy in alcoholic grape beverages

Plamen Chorbadzhiev^{1,2}, Dessislava Gerginova², Svetlana Simova²

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²Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

Wine is a popular alcoholic beverage and a medicine. Its composition depends on several factors. Bulgaria's Neolithic sites have grape seeds dating back to 6000 BC. The Thracians, known for their "sweet wine of Thrace," lived in the region around 1000 BC. Bulgarian wine is renowned for its aroma, flavor, and high quality. As wine ages, chemical reactions enhance its flavor. Grape ales combine beer brewing techniques with winemaking. They involve adding grape juice, must, or whole grapes during fermentation. This results in a beer with wine-like flavors and aromas.

The chemical profile of young and aged wine was determined using ¹H NMR spectroscopic analysis to study the aging process. The method was also applied to grape ale, a relatively new type of beer introduced in Italy in 2006. Quantification of the identified compounds was carried out, with further application of statistical methods in the differentiation of the grape products.

Acknowledgements. This work was supported by the Bulgarian National Science Fund, Project KP-06-M79/2. Research equipment purchased by Project No BG05M2OP001-1.002-0012 and part of the Distributed Research Infrastructure INFRAMAT, supported by the Ministry of Education and Science, were used in this investigation.

Enhanced heating systems for fluidized bed reactors: innovations and applications

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²Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

In a fluidized bed, a fluid (gas or liquid) is circulated through solid particles, making the mix behave like a fluid. This technology is increasingly used in industrial processes like shaping, coating, and drying due to enhanced heat and mass transfer. Traditional heating relies on preheating the fluidizing gas via convection. An alternative is inductive heating, which uses electrically conductive, inert particles within an electromagnetic field. This method transfers heat directly to the bed material without heating the incoming fluid. Inductive heating offers efficient, rapid heat exchange, allowing precise temperature control, improved energy density, and enhanced product quality. This study outlines the principles of inductively heated fluidized beds and explores potential applications.

Poster 8:

Development of a measurement method for determining the drying kinetics of volatile water and alcohol components in solids

Boyana Kostadinova¹, Vesselin Idakiev¹, Torsten Hoffmann²

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²Institute of Process Engineering, Otto-von-Guericke-University Magdeburg, Germany

This study investigates the drying kinetics of water and ethanol in porous γ -Al₂O₃ particles using a thermal drying process in a magnetic suspension balance under atmospheric pressure. Superheated steam served as the drying medium, introducing sufficient energy to fully desorb volatile components even from the smallest pores. The porous γ -Al₂O₃ particles, 1.8 mm in diameter, were saturated with varying concentrations of water-ethanol mixtures. γ -Al₂O₃, known for its high mechanical strength and large internal surface area, is widely used as an adsorbent and catalytic material. The study highlights the complex interactions between water and ethanol at the molecular level, which influence the adsorption behavior within the porous matrix. The experimental results provide insights into the physicochemical properties of γ -Al₂O₃, supporting its potential for broader industrial applications.

3D design and research of a continuously operating bioreactor with mechanical agitation and aeration

Radoslava Ivanova, Desislava Mutafchieva, Vesselin Iliev

University of Chemical Technology and Metallurgy, Sofia, Bulgaria

The aim of this study is to analyze a continuously operating bioreactor with mechanical agitation and aeration for the production of L-glutamic acid and to numerically investigate its hydrodynamic and thermomechanical characteristics within the ANSYS Workbench environment. To achieve this, a bioreactor was dimensioned and standardized with operational parameters ($D = 3$ m; $H = 9$ m; gas flow rate for aeration 0.497 m³/s and impeller speed: 0.158 rad/s). Hydrodynamic (ANSYS CFX) and structural (Static Structural) simulations were performed. For this purpose, a geometric model of the bioreactor was created, with a mesh consisting of 1,529,823 elements and 262,279 nodes. The hydrodynamic analysis revealed a linear increase in pressure with increasing fluid depth in the bioreactor, as well as a uniform distribution of gas content, which becomes uneven when the impeller speed is reduced.

The structural simulation shows that the stresses under extreme operating conditions are significantly higher than those under normal operating conditions. Although a lower safety factor is allowed under extreme loads, there arises a need to increase the size of the supports.

From the interpretation of the obtained numerical results, it can be concluded that the continuously operating bioreactor with mechanical agitation and aeration is suitable for the production of L-glutamic acid.

Poster 10:

Study of the mixing process of two immiscible liquids

Vasil Kostov, Desislava Mutafchieva, Vesselin Iliev

University of Chemical Technology and Metallurgy, Sofia, Bulgaria

A model has been created using ANSYS CFX for the computer simulation of a reactor with a paddle impeller for mixing methyl orange and liquid paraffin. To verify the model, a laboratory experiment was conducted in a cylindrical vessel with dimensions of 200 mm diameter, 290 mm height, and an impeller with 4 blades, each 33 mm high and 28 mm wide, positioned 20 mm from the bottom of the vessel. Under maximum property differences between the two liquids, and with the impeller speed varying from 0 rpm to 500 rpm over a four-second period, the movement of the liquids became steady after 25 seconds. When the dynamic viscosities of the liquids were closer in value, steady-state flow was achieved after 30 seconds. Successful verification of the model was achieved with a primary mesh size of 25 mm. Additional investigations were carried out on the size of the reflective baffles, and the optimal dimensions were determined to be 1 mm thickness and 28 mm width.

When evaluating the adequacy of the created model, it was found that turbulent viscosity could serve as a criterion for showing the effectiveness of mixing.

The developed model can successfully be used for computer simulation of the mixing process of two immiscible liquids with densities and viscosities corresponding to those used in the chemical industry.

Poster 11:

Optimization of the dispersion process in the production of industrial coatings

Esin Paleva, Desislava Mutafchieva, Alexander Kirilov

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This study focuses on the optimization of the dispersion and milling processes in the production of epoxy protective coatings. The goal is to investigate the impact of different viscosity levels on the efficiency of these processes, by testing three variants of a standard starting formulation with low, medium, and high viscosity. Dispersion was performed using a high-speed dissolver, while the subsequent milling was carried out with a pearl mill, utilizing zirconium beads to achieve high kinetic energy, which aids in the effective deagglomeration of the particles. In addition to the mill speed, the type of grinding media also has a significant impact on milling efficiency. The denser the material of the grinding media, the higher the kinetic energy, which leads to better milling. By controlling parameters such as dispersion speed, viscosity, density, and temperature, defects such as agglomeration and delamination are reduced, while production efficiency is simultaneously improved. The results show that proper management of these parameters leads to a significant improvement in the homogeneity and stability of the coatings, providing practical guidelines for optimizing the production process.

The study also explores innovative dispersion approaches, such as ultrasonic dispersion and microfluidic technologies, which offer prospects for further optimization and economic efficiency in the industrial production of coatings.

Poster 12:

Green solvent extraction and separation of 4f-ions with chelating ligands: mechanistic modelling

Maria Atanassova, Nina Todorova, Gabriel Stoimenov, Katrin Chavdarova, Ilina Todorova

Department of General and Inorganic Chemistry, University of Chemical Technology and Metallurgy,
Sofia, Bulgaria

The investigation aims at a rational search for unfamiliar, high yield and eco-efficient processes to extract and separate valuable metals via sustainable extraction that embodied 4f-ion high-performance behaviors. Unfortunately, end-of-life recycling rates for all rare earth elements are below 1%. Study of the liquid-liquid extraction of 4f-ions with a series of chelating ligands of 4-acylpyrazolones family (~5) is presented employing ionic liquids and typical organic diluents: 14 in number. Another step forward is to develop a non-aqueous process for switchable extraction and separation upon addition of ethylene glycol, i.e. boost of two immiscible organic phases, comparing to traditional aqueous solutions. The competitive solvent extraction of 18-f ions has also been conducted to evaluate the 4f-intagroup selectivity as well as between 4f/5f-ions. Furthermore, the composition of the extracted Gd-species in ionic liquid solutions was investigated by EPR, NMR, IR, DTA-TG-MS and UV-Vis spectroscopies in order to gain a deeper understanding of the influence of chemical nature of organic oil media and ligand's functional groups over Gd complexation.

Poster 13:

A study on encapsulation of lavender oil essence in zeolite and bentonite-based matrices

J. Mateeva, O. Musa, S. Djambazov, A. Yoleva

University of Chemical Technology and Metallurgy, Sofia, Bulgaria

In the present research, the encapsulation of the oil essence of lavender in the matrices of natural zeolite and alkaline activated bentonite have been studied in order to preserve the aroma of the oil essence for a long time. Zeolite was crushed and fractionated to a particle size of 1 to 2.5 mm and the bentonite was granulated with an agitating teeth granulator to spherical granules with the same. The weight change of the matrices loaded with lavender oil essence (in the amounts 5, 15 and 30 mass%) has been monitored after a certain period in the air for 1, 2, 7, 9, 14 and 60 days at room temperature. To prove the retention of the oil in the matrices the samples were analyzed by using XRD, FTIR, DTA and TG analyses. Zeolite and bentonite have been found to be suitable natural aluminosilicate matrices for the encapsulating of the essential oils in order to preserve the aroma for longer. Bentonite shows better results of the two materials, thanks to its layered structure, which allows the insertion of the organic oil molecules in it, passing into organobentonite, preserving the aroma of the oil for a longer time and preventing its degradation.

Poster 14:

Development of multicomponent glasses for application as a glazing layer on dental zirconia

Tina Tasheva, Albena Yoleva, Stoyan Djambazov, Adriana Batsova

University of Chemical Technology and Metallurgy, Sofia, Bulgaria

This study presents the development of multicomponent glasses for glaze layers for dental yttria-stabilized tetragonal zirconia (Y-TZP). The samples were melted in the temperature range of 1 250–1 400°C and were cast in water to obtain a frit. The frits were grounded to a powder with a particle size of less than 40 µm. To study the crystallization tendency of melted glasses, they were thermally treated at 800°C and X-ray diffraction analyses were performed for both types of samples. The structure of the glasses was investigated by the Fourier-transform infrared spectroscopy. The thermal expansion coefficient, CTE, the glass-transition temperature, T_g, and the softening temperature, T_s, were defined. To test the glaze layer on zirconia ceramic, glass powders with different compositions were mixed with modeling fluid and applied on zirconia specimens and then fired at 800°C in a vacuum dental furnace. Scanning electron microscopy, SEM, was used to observe a cross-section of the glass–ceramic contact on a glazed zirconia ceramic specimen. Glass with the highest content of alkaline oxides is characterized by the closest CTE to zirconium ceramics (10.10–6 K⁻¹), the greatest transparency and good fluidity, and shows good adhesion to the zirconia. The glaze layer is homogeneous without cracks, pores, and crystals.

Guerbet condensation of 1-butanol over zeolite catalysts

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Synthetic liquid fuels based on waste biomass sources are becoming a topical issue to limit the greenhouse effect of CO₂ coming from fossil fuels. The development of catalysts with optimised microstructure for the Guerbet condensation of primary alcohols (bioethanol and biobutanol) into a mixture of liquid fuels (alkanes, alkenes) and higher alcohols is an important issue in sustainable chemistry studies. We explore the physicochemical properties and catalytic activity of Mg and Li containing samples supported on L type zeolite. Gas-phase coupling of 1-butanol was investigated in a flow reactor at 400 oC and atmospheric pressure. The hydrothermal synthesis of the pure zeolite L was carried out from the initial gel composition of 20 SiO₂:Al₂O₃:10 K₂O:400 H₂O. Mg and Li (0.6 mmol/g) were applied by wet impregnation using Mg(NO₃)₂·6H₂O (Mg/L catalyst) and LiNO₃ (Li/L catalyst), respectively. The catalysts were dried, calcined at 400 °C and characterised by using a combination of N₂ adsorption-desorption isotherms, XRD, FT-IR, XPS, TPD-CO₂ and TPD-NH₃. The BET surface area of the L zeolite was 274 m²/g. The micropore area and volume was 96 m²/g and 0.05 cm³/g, respectively. With regard to the Mg/L and Li/L catalysts, the impregnation of Mg and Li decreased the surface area and significantly reduced the micropore volume, while the total pore volume and pore size increased. XRD and FTIR results showed no major changes in the crystal structure of the modified zeolite. The Li/L had more than 3-fold higher C-C coupling activity than the Mg/L. Moreover, this catalyst formed preferentially Guerbet derivatives and C8 hydrocarbons and had a higher concentration and strength of medium base sites according to TPD-CO₂. Calcination at 400 oC of Mg/L and Li/L samples resulted in the formation of a highly dispersed Mg and Li oxide phase with weakly acidic properties. These exposed sites slightly enhanced the side reaction of butanol dehydration. Small quantities of butanal, 4-heptanone and C7 hydrocarbons were detected in all reaction products.

Poster 16:

Technology and installation for purification and neutralization of acid gases

D. Kolev

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During the industrial production of sensors in the company Sensata Technologies Bulgaria air pollution is produced in the production premises. The company's production is located in the territory of the village Tsaratsovo, municipality Maritsa. The built respiration system with a capacity of 6000 m³/ hour captures them. Contaminations are observed in both gas and liquid phase. The pollutants are hydrogen acetate (HAC), hydrogen fluoride (fluorine HF), nitric acid (HNO₃), and silver nitrate (AgNO₃). The concentrations of the individual components vary over time. The gases have a pronounced acidity.

The proposed method for gas purification is absorption with sodium base solution (NaOH) performed in a packed bed column. The column is loaded with an ordered honeycomb packing with an inscribed circle radius of 20 mm and a height of 60 mm. Above this is a redistribution packed of stacked Raschig rings 50 mm in diameter. The Raschig rings are beveled at 16 degrees. The concentration of the solution is automatically maintained within a range of 8-10 Ph. The figures and photographs in the poster show the complete plant layout as well as the completed industrial plant. According to the samples carried out, the gases coming out of the plant meet the environmental criteria.

Poster 17:

Academic English and German: Chemical and Biochemical Engineering

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Technical and scientific translation requires both very good knowledge of the languages from and into which it is being translated, as well as an understanding of the meaning of the text being translated.

The proposed project aims to improve professional foreign language training in the field of chemical and biochemical engineering for students from UCTM with a strong interest in English and German.

The project is focused on:

1. Academic English and German commonly used vocabulary in:

- Lectures and scientific discussions;
- Presentation of scientific data;
- Conferences, meetings and other scientific forums;
- Publications and scientific reports;
- Workshops and other practical training courses.

2. Technical and scientific translation of specialized texts and commonly used terms and phrases in the field of Chemical and Biochemical Engineering between Bulgarian, English and German

3. Advanced Grammar Course in English and German

4. Consecutive (and simultaneous) translation between Bulgarian, English and German in the field of Chemical and Biochemical Engineering at:

- Fairs and advertising industry events;
- Business and professionals' meetings;
- Visits of specialists and non-specialists to chemical and biotechnological companies;
- Presentations of new technical devices and technologies;
- Training of personnel in the chemical and biotechnological industry.

Poster 18:

An integrated novel approach to the sustainable recovery of bioactives from Croton lechleri twigs

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Croton lechleri tree growing in Mexico, Colombia, Venezuela, Ecuador, Peru, and Brazil, etc. is known for the production of red latex called Dragon's blood. It has been used for centuries in traditional medicine owing to its diverse biological activities. From all parts of the C. lechleri plant, the twigs are among the least studied. This investigation is focused on a comparison of the efficiency of traditional (Soxhlet) and advanced green techniques (pressurized liquid extraction and supercritical fluid extraction with co-solvent) regarding yield, total phenolic content and antioxidant activity of the extracts recovered. Furthermore, extracts biological activity was analyzed using both normal and malignant melanoma skin cell lines. It was demonstrated that the extracts exhibited significant cytotoxic activity, particularly against malignant melanoma cells, and promising antioxidant and wound-healing properties.

The findings of this investigation offer a new perspective for the sustainable transformation of C. lechleri twig biomass, generally considered as waste, into valuable phytochemicals for various industries, including pharmaceuticals, nutraceuticals, and cosmetics.

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Poster 19:

On the influence of Soxhlet operating conditions on extract yield of Cornelian cherry stones – a neglected waste

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Cornus mas L., commonly known as Cornelian cherry, is a small tree producing fleshy and edible red fruits. It is native of temperate zones, from Central to Southern Europe and Asia. Some countries like Turkiye and China are known to cultivate Cornelian cherry and use its fruits for consumption and oil production, as well as for medicinal purposes. However, Bulgaria is not a Cornelian cherry cultivar.

Decoctions, as well as organic solvents extracts of *C. cherry* fruits have been extensively studied and their chemical composition identified. Still, the information regarding *C. cherry* stones is quite scarce.

This study is a first step towards determining the potential of the stones as a viable source of valuables, starting with exploration of the influence of the operating conditions of a traditional method like Soxhlet on extract yield. In particular, the type of solvent and hydromodule used were examined. Our preliminary results showed that the highest yield was obtained with ethanol, followed by water, while the lowest was obtained using n-hexane. The influence of the hydromodule is more pronounced in the case of water extraction as compared to that with ethanol.

Synthesis and characterization of heterocyclic hydrazones with biological application

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Heterocyclic compounds are of significant importance in both fields of medicine and organic chemistry. Benzimidazole is one of the oldest known nitrogen heterocycles and was first synthesized by Hoebrecker [1], and subsequently by Ladenberg and Wundt [2, 3]. Approximately 50 derivatives of 2-aminobenzimidazoles occurs in the structure of many clinically useful drugs with anticancer, antiviral, antibacterial, anti-parasitic and antihistamine properties [4]. Some of them as albendazole, omeprazole, lansoprazole, bendamustine, nocodazole etc. have found application in medicinal practice.

Herein we report the synthesis of a series of 2-aminobenzimidazolyl hydrazones, achieved by a multi-step reaction pathway. The target compounds were obtained by a reaction of condensation with various hydroxyl and methoxyl-acetophenones. The structure of the hydrazones was characterized by quantum-chemical calculations using the Gaussian 09 program. Furthermore, several mechanisms of radical scavenging activity (HAT, SET and SPLET) were evaluated in polar and non-polar medium.

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Poster 21:

Modelling of the extraction kinetics of *Melissa officinalis*

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Efficient extraction of phenolic compounds from plants is vital for optimizing industrial applications. Solid-liquid extraction processes are influenced by the structural complexity of plant materials, solvent type, and temperature. This study focuses on the extraction of phenolic compounds from *Melissa officinalis* (lemon balm) to identify optimal conditions for yield and efficiency.

Extraction kinetics were studied in a stirred vessel using deionized water, 40% and 70% ethanol at 30°C and 40°C. Agitation was controlled to maintain internal diffusion-limited conditions, and total phenolic content was measured spectrophotometrically. Effective diffusion coefficients were determined using two methods: the Standard Function Method (SFM) and the Regular Regime Method (RRM).

While SFM assumes constant diffusion coefficients, RRM accounts for variations due to structural changes in the solid phase during extraction. Results indicated minimal differences in diffusion coefficients between solvents at similar temperatures. The RRM produced more accurate fits to experimental data, highlighting the importance of accounting for dynamic diffusion rates.

Optimal extraction conditions for phenolic compounds from *Melissa officinalis* were achieved at 40°C using 40% ethanol. The study demonstrates the reliability of RRM for modelling extraction systems with variable diffusion coefficients, providing valuable insights for industrial-scale applications.

Acknowledgements: This work was supported by the contract 239-14 at NIS-UCTM, Sofia, Bulgaria.

Poster 22:

Testing of a conventional method for the analysis of gold from gold-bearing copper concentrates at "Ellatzite - Med" JSC

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"Ellatzite-Med" JSC – a high-technology mining company extract and concentrate porphyry-copper and gold-bearing ores from the trove "Ellatzite". For analysis of this type of objects – inhomogeneous with low gold contents, it is necessary to apply of a method for gold analysis which includes dissolving a sample of gold-bearing concentrate with acids, subsequent extraction with a selective solvent – Methyl isobutyl ketone (MIBK) and measuring the result by atomic absorption spectrometer – AAS Agilent 240.

Acknowledgements

This work was supported by the contract 239-14 at NIS-UCTM, Sofia, Bulgaria.

The results of certified reference materials and samples from the production process obtained show good precision, standard deviation of the analysis for each sample being less 5%.

This method fully meets the range of sought-after gold contents in copper concentrate, which makes it suitable for use in the practice of laboratories that are part of the mining company.

Poster 23:

Spontaneous deposition of Pd-Ag particles on carbon screen printed electrodes

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Two types of carbon screen-printed electrodes, consisting of carbon nanofibers (CNF) and single-walled carbon nanotubes (SWCNT), were investigated for bimetallic modification with Pd and Ag through a spontaneous deposition process. By determining the suitable pre-reduction potentials required for the spontaneous metal deposition process, it was found that the processes of consequent electrode reduction and immersion in solutions of metal ions (Pd^{2+} and Ag^+) allow the combined deposition of both metals. Additional characterizations obtained by SEM and EDX analyses of the deposited metal particles on the carbon surface show that bimetallic nanoparticles are deposited, with average sizes between 13 nm for CNF and 24 nm for SWCNT.

Poster 24:

Water purification from 1,2-Dichloroethane and 1,2-Dibromoethane using some bacterial strains

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Bacterial cells of the strains *Xanthobacter autotrophicus* GJ 10, *Klebsiella Oxytoca* VA 8391 and *Bradyrhizobium japonicum* 273 successfully degraded halogenated hydrocarbons at low initial concentrations up to 0.1 g/l. When 1,2-dibromoethane concentration is 0.3 g/l, complete biodegradation was obtained using cells of the bacterial strain *Bradyrhizobium japonicum* 273 immobilized on granular polymer particles. When a constant electric field was applied, the concentration of chloride and bromide ions in the medium reached stoichiometric values regardless of the initial concentration of the contaminant. The best results were obtained in the bioelectrochemical potentiostatic mode at a potential of 0.8029 V/S.H.E.

Acidic Lignocellulosic Hydrolysates: New achievements in their detoxification by liquid – liquid extraction with ionic liquids

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This study examines acidic lignocellulosic hydrolysates (LCH) from the perspective of their detoxification of the inhibitory substances (produced in the hydrothermal pretreatment) to become biocompatible media for enzymatic hydrolysis and microbial fermentation. Inhibitors include the inorganic acid catalyst, most commonly H₂SO₄, aliphatic carboxylic acids, furans and aromatic (phenolic and non-phenolic) compounds. The traditional methods applied for their removal from LCH, such as alkali treatment, adsorption with AC or resins, and liquid – liquid extraction with organic solvents, are discussed with their advantages and drawbacks. For the purpose of complex detoxification of LCH, some ionic liquids (ILs), instead of classical organic solvents, emerge as more promising and benign extractants. Compared to molecular organic solvents, the nature of coordinating ILs, such as phosphonium phosphinate or carboxylate, suggests biocompatibility and high extraction capacity. These characteristics arise from the high hydrophobicity and stability of both ions of these ILs and from the strong H-bonding basicity of their anions.

Our developments reveal these ILs as the best extractants for complex detoxification studied both on a multicomponent model solution and a real rice straw LCH. Detoxified LCH have been tested and shown to have no detrimental effect on the cellulytic enzymes used in the enzymatic hydrolysis step.

Partial dealcoholization of red wine Mavrud by nanofiltration

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Membrane nanofiltration technology is an efficient method for wine dealcoholization and concentration of various bioactive compounds and has a vast number of applications in wine production. In order to obtain optimal features of the obtained products, both the parameters and the mode of filtration, as well as the characteristics of the used filtration membrane, are of great importance. In this study, nanofiltration of the native Bulgarian red wine Mavrud via MaxiMem Prozesstechnik GmbH filtration system, completed with polymer membranes was performed. Rejection coefficients of ethanol and selected wine components were measured and their increase with applied pressure (10 to 50 bar) was observed. Cross-flow flat sheet nanofiltration with polymer membranes was performed in concentration and diafiltration mode. Partial dealcoholization (5-8% EtOH) was obtained with good preservation of the remaining composition. Depending on the degree of dealcoholization and the characteristics of the membranes, a loss of 0 to 24% anthocyanins, 8 to 19% polyphenols and 2 to 30% ORAC activity was observed.

Waste coffee grounds - millions of tons of waste or a source of valuable substrate for high value-added products?

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Coffee is one of the most widely consumed beverage. International Coffee Organisation reported that the global coffee industry worth \$495.50 billion as of 2023. The processing of coffee produces over two billion tons of solid wastes including husk, pulp, silverskin, defective beans, and spent coffee grounds. Over the last 5–10 years, the circular economy has gained increasing interest. The use of coffee waste is based on its promising chemical composition.

Spent coffee grounds (SCG) contain oils, lipids, triglycerides, and fatty acids, along with insoluble carbohydrates like cellulose, hemicellulose, and various indigestible sugars.

Nowadays, where concerns about industrial pollution are growing, there's a significant focus on using often ignored resources like spent coffee grounds.

The aim of our work is the utilization of SCG by extracting their reducing substances to serve as substrate for microbial production of lactic acid. Protocols for extraction of reducing sugars and purification of hydrolysis from inhibitors were applied.

Lactobacillus plantarum 2HS strain was selected to fulfill the objective. The results showed 21 g/L lactic acid derived from 18 g/L substrat.

This work strengthens the position of SCG as a reliable source of sugars for the production of high value added products.

Multi-parameter optimization of polymer nanocomposites under combined loading

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In the present study, the influence of the geometry (layer thicknesses and length) and the magnitude of thermo-mechanical loading on the delamination in polymer nanocomposites, is theoretically investigated. The analytical solutions for the interface shear stress (ISS) in the structure are obtained, based on the application of 2D stress-function method and minimization of the strain energy. The theoretical criterion for delamination in the interface layer, based on the ISS model solutions is formulated, including the structure geometry and loadings as parameters. A multi-parameter optimization problem including this criterion is defined and solved. By simultaneously varying these parameters, the safety intervals of the parameters (without delamination) in the considered nanocomposite structures are obtained, for several case studies with different 2D nanomaterials. It was found, that the magnitude of the applied load mainly affects the magnitude of the ISS. Layers thicknesses mostly affect the type of ISS solution, especially the substrate thickness. The effect of layer length on ISS is weaker than that of layer thickness at a fixed load. The influence of temperature loading on the delamination appears to be important in cases where the magnitude of the mechanical load is close to the limit values for which delamination is observed.

Acknowledgement

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UV-assisted grafting as a tool for surface modification of polyethersulfone nanofiltration membranes

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With the development of macromolecular surface science, surface grafting polymers, also known as polymer brushes, have become an important approach to modify or functionalize the surface of materials. Graft polymerization induced by UV irradiation is a commonly used polymer membrane surface treatment method due to its high efficiency, simplicity, and distribution of grafted chains near the surface without damaging the bulk membrane structure. In this work, nanofiltration polyethersulfone membrane properties were modified by UV-assisted grafting of a hydrophilic monomer, namely N-isopropylacrylamide (NIPAAm), when using benzophenone as photoinitiator.

Green eco-friendly UV chemometric methods for simultaneously quantifying of four component anti-migraine drug formulation Paracofdal

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In the last decades, considering the green chemistry perspective and improving the environmental impact of quality control labs direct techniques with less hazardous solvents, less waste production and less energy consumption were developed for simultaneous analysis of drug formulations.

These features can be achieved by means of using spectroscopic technique, because of being simple, robust and inexpensive, and due to their capability of generating first order data. In order to exploit that data, generated by HP8452 UV-Vis Agilent multivariate approaches (PLS and MCR ALS) needs to be explored.

Poster 31:

Total antioxidant activity and total phenolic concentration in plant raw material

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Antioxidants are compounds that inhibit oxidation (usually occurring as autooxidation), which is the chemical reaction that produces free radicals. They are considered the organism's first choice of defense, present in moderately low concentrations with the task to transform the reactive species into more stable molecules. Naturally occurring phenols are of interest due to their antioxidant activity.

Within the framework of the current project, nine plant raw materials were studied to determine their total antioxidant activity and total phenolic concentration.

The total antioxidant activity was assessed using the DPPH method, with the highest value observed in lemon balm (*Melissa officinalis*). For three of the plant raw materials (ashwagandha, passionflower, and valerian), practically no antioxidant activity was detected. The total phenolic concentration was determined using the Folin-Ciocalteu method. A similar trend to that of antioxidant activity was observed: lemon balm stood out with the highest phenolic concentration, while the presence of total phenols in ashwagandha, passionflower, and valerian was almost negligible.

Based on the results for antioxidant activity and total phenolic concentration, lemon balm was selected as the model raw material for characterizing the kinetics of the extraction process.

Acknowledgements: This work was supported by the contract 239-14 at NIS-UCTM, Sofia, Bulgaria.

Poster 32:

Biogas - an alternative to fossil fuels

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In the presented poster, various methods for biogas production and its potential applications are discussed. Different organic wastes, their processing, and the loading scheme into the bioreactor leading to biogas generation are examined.

Poster 33:

Application of membrane filtration and spray drying technologies for the recovery of antioxidants from spent lavender

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This study investigates the application of membrane filtration for the valorization of spent lavender generated during essential oil production, focusing on the recovery of natural antioxidants. A 40% ethanol solution was used to extract bioactive compounds such as rosmarinic acid, caffeic acid, and luteolin, which have significant applications in the food and pharmaceutical industries. Membrane filtration was conducted in batch mode using the PA-Urea-TFC X201 membrane (TriSep, USA), under controlled conditions of room temperature and a transmembrane pressure of 20 bar. The resulting fractions were then subjected to spray drying, and the biological activity of the extracts, nanofiltrated fractions, and final powders will be evaluated to validate the efficacy of the proposed methodology.

This research aims to demonstrate the potential advantages of employing nanofiltration and spray drying technologies in the treatment of spent lavender, providing a sustainable solution for waste reduction and the recovery of valuable bioactive compounds.

Acknowledgements: This work was supported by the University of Chemical Technology and Metallurgy Science Fund "Research Investigation" (Project № 239-01), Bulgaria

DNA fragmentation and apoptosis induction by polymer nanocarriers loaded with anticancer podophyllotoxin or juniper extracts

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Nanotechnology offers alternative approaches to overcome limitations of the conventional anti-cancer therapy. Hydrophobic bioactive components can be included in the core of nanocarriers, based on amphiphilic copolymers. As a result, a water-soluble product is obtained, aimed at improvement of the bioavailability, facilitation of the excretion, reduction of the toxicity of poorly water-soluble substances. In this study, new polymer nanosized micelles, loaded with anticancer podophyllotoxin (PPT) or PPT-containing leaf extracts of *Juniperus horizontalis* or Grey Owl juniper were obtained and their mechanism of antiproliferative activity was investigated.

The amphiphilic MPEG-b-PLA [monomethoxypoly(ethylene glycol)-block-poly(D,L-lactide)] diblock copolymer self-assembled into nanosized particles (average diameter of around 45 nm). Physico-chemical characteristics of empty and loaded nanocarriers were determined by dynamic light scattering, transmission electron microscopy etc. High encapsulation efficiency (74-98%) was detected for micelles loaded with PPT or juniper extracts.

The antiproliferative properties of micelles loaded with PPT or *Juniperus horizontalis* extract were studied in detail. Efficient DNA fragmentation, cell cycle arrest, growth inhibition and apoptosis induction in A-431 epidermoid carcinoma and HaCaT normal keratinocyte cells were detected by MTT test, Hoechst staining, FACS, Comet assay and fluorometric analyses.

The newly obtained polymer micelles loaded with PPT or PPT-containing leaf extracts have potential application in the prospective nanomedicine.

Acknowledgements: The authors thank for support of contract № 37-2016 with the Arnold Arboretum, Harvard University, Boston, MA, USA for delivery of juniper species; Bulgarian Ministry of Education and Science, Bulgarian National Roadmap for Scientific Infrastructures 2020–2027, Scientific Infrastructure on Cell Technologies in Biomedicine (SICTB) contract D01-361/2023.

Evaluation of Heterogeneous Environmental Catalysts Using Temperature-Programmed Desorption, Reduction, and Oxidation – Methods and Applications

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The key role in solving many environmental problems in catalytic science plays developing new, highly active, and stable catalysts for zero-waste technologies and processes in industry and transport.

The thorough understanding of the surface structure and surface chemistry of the catalytic material requires for efficient utilization of catalysts. The focus of this study is to present some aspects of the application of the temperature-programmed analysis technique for the investigation of heterogeneous catalysts at the Institute of Catalysis in the Bulgarian Academy of Sciences.

There are three reactions that are studied as a function of temperature: reduction, oxidation, and desorption. Temperature-programmed desorption (TPD) is used to analyze adsorbed species (which might be deliberately introduced by a preadsorption step) in inert atmospheres. Temperature-programmed reduction (TPR) and temperature-programmed oxidation (TPO) probe the susceptibility to reduction and oxidation, respectively, and are carried out in the presence of hydrogen in the case of TPR and oxidants such as oxygen or carbon dioxide in the case of TPO.

The results of the described techniques can be useful for researchers to effectively optimize the performance of catalysts and develop novel materials with enhanced properties.