SICHEM 2025

BOOK OF ABSTRACTS

06 – 07 November 2025

Romanian Chemical Engineering Society

Romanian Chemical Society

Academy of Technical Sciences – Chemical Engineering Section

National University of Science and Technology Politehnica Bucharest,
Faculty of Chemical Engineering and Biotechnologies
(Departments of Chemical and Biochemical Engineering and Science and Engineering of Oxide Materials and Nanomaterials)

Scientific Committee

Șerban AGACHI – Babeș-Bolyai University of Cluj, ASTR
Petru ILEA – Babeș-Bolyai University of Cluj
Csaba PAISZ – Babeș-Bolyai University of Cluj
Alexandru OZUNU – Babeș-Bolyai University of Cluj
Mircea Vasile CRISTEA – Babeș-Bolyai University of Cluj
Cristian Calin CORMOȘ – Babeș-Bolyai University of Cluj
Liana Graziella TURDEAN – Babeș-Bolyai University of Cluj
Valeria HARABAGIU – Institutul Chimie Macromoleculara Petru Poni Iași
Maria GAVRILESCU – Gh Asachi Technical University of Iași, ASTR
Dan CAȘCAVAL – Gh Asachi Technical University of Iași
Ilie SIMINICEANU – Gh Asachi Technical University of Iași, ASTR
Ioan MĂMĂLIGĂ – Gh Asachi Technical University of Iași
Gabriela LISA – Gh Asachi Technical University of Iași
Silvia CURTEANU – Gh Asachi Technical University of Iași
Nicolae VASZILCSIN – Politehnica University of Timișoara, ASTR
Delia PERJU – Politehnica University of Timișoara, ASTR
Teodor TODINCĂ – Politehnica University of Timișoara
Gabriela-Alina DUMITREL – Politehnica University of Timișoara
Viorica POPESCU – Ovidius University of Constanța
Claudia MUNTEAN – Ovidius University of Constanța
Ionela POPOVICI – Ovidius University of Constanța
Timur CHIS – Petroleum and Gas University of Ploiești
Ion ONUȚU – Petroleum and Gas University of Ploiești
Dorin BOMBOS – Petroleum and Gas University of Ploiești
Dragos Mihael CIUPARIU - Petroleum and Gas University of Ploiești
Denisa NISTOR – Vasile Alecsandri University of Bacău
Mihaela DONI – INDCP ICECHIM București
Florin OANCEA – INDCP ICECHIM București
Andrei SARBU – INDCP ICECHIM București
Philippe MICHAUD – Clermont Auvergne INP, SIGMA Clermont
Fabrice GROS – Clermont Auvergne INP, SIGMA Clermont
Cristhophe VIAL – Clermont Auvergne INP, SIGMA Clermont
Mihail BĂRBOIU – European Institute of Membranes of Montpellier
Jose Marcano SANCHEZ – European Membranes Institute of Montpellier
Inmaculada Rodriguez RAMOS – Ins. of Catalysis and Petrochemistry of Madrid
Ecaterina ANDRONESCU – NUST Politehnica Bucharest, ASTR
Horia IOVU – NUST Politehnica Bucharest
Cristina ORBECI – NUST Politehnica Bucharest
Ioan CĂLINESCU – NUST Politehnica Bucharest
Gheorghița JINESCU – NUST Politehnica Bucharest, ASTR
Anicuța STOICA – NUST Politehnica Bucharest
Gheorghe MARIA – NUST Politehnica Bucharest, Ro Academy
Tănase DOBRE – NUST Politehnica Bucharest, ASTR
Sorin BÎLDEA – NUST Politehnica Bucharest
Sorin JINGA - NUST Politehnica Bucharest
Anton FICAI – NUST Politehnica Bucharest

Table of Contents

Plenary 4
A – Chemical and biochemical engineering (CBE).....31
1. Keynotes 31
2. Oral presentations 33
3. Poster presentations 58
B – Applied organic, inorganic, and supramolecular chemistry in process engineering (AOISCPE) 107
1. Keynotes 107
2. Oral presentations 110
3. Poster presentations 122
C – Biomaterials and composites in chemical and biochemical applications (BCCBA) 139
1. Keynotes 139
2. Oral presentations 141
3. Poster presentations 164
D – Green applied chemistry and agro-resources valorization (GACARV) 190
1. Oral presentations 190
2. Poster presentations 204
AUTHORS INDEX……...……..232

BOOK OF ABSTRACTS

SICHEM – 2025

Plenary

PL01 ELINKING CATALYST DEVELOPMENT AND PROCESS DESIGN: APPLICATION TO BUTADIENE MANUFACTURING FROM ETHANOL

Alexandre C. Dimian*

Technical Sciences Academy of Romania, 26 Dacia Bld, 030167, Bucharest, Romania

Abstract: *Catalyst research is a key innovation driver in the transition toward a chemical industry based on renewable raw materials and waste. This presentation highlights the strong interconnection between industrial catalyst development and chemical process design. Systematic methods from Process Systems Engineering (PSE), combined with the capabilities of Computer-Aided Process Engineering (CAPE) tools, enable early-stage assessments of technical feasibility and economic viability—even when only small amounts of catalyst are available. However, accurate predictions require detailed information on product distribution and reaction kinetics. This approach is illustrated through original research conducted by the author and collaborators on sustainable ethanol-to-butadiene (ETB) processes.*

Key words: Ethanol-to-Butadiene process, Catalyst research, Process Systems Engineering, Computer-Aided Chemical Engineering, Chemical Process Design

Introduction: Currently, 1,3-butadiene (BD) is produced exclusively from fossil-based sources. Transitioning to renewable raw materials is an urgent priority. Ethanol—whether biosourced or synthetic—offers a promising alternative. Major companies are actively developing industrial processes based on ethanol, and Romania has the potential to benefit significantly from this opportunity. This paper presents research conducted by the author and co-workers over the past four years. Two ethanol-to-butadiene (ETB) process routes are considered: a one-stage process and a two-stage process.

Reaction schemes:

R1: $2\ C_2H_5OH \rightarrow CH_2{=}CH{-}CH{=}CH_2 + {}_2H_2O + H_2$ $\Delta H(R,298) = 95.4$ kJ/mol

R2a: $C_2H_5OH \rightarrow CH_3CHO + H_2$ $\Delta H(R,298) = 68.6$ kJ/mol

R2b: $C_2H_5OH + CH_3CHO \rightarrow CH_2{=}CH{-}CH{=}CH_2 + {}_2H_2O$ $\Delta H(R,298) = 31.5$ kJ/mol

In the one-stage process, the catalyst (Lebedev type) must perform both dehydrogenation and aldol condensation. In contrast, the two-stage process uses separate catalysts tailored for optimal selectivity. Most ETB catalysts suffer from the formation of numerous by-products and impurities, which reduce carbon yield. The two-stage process can achieve yields over 80%, while the one-stage process typically reaches around 70%. Although recent research has focused on improving the one-stage process, progress has been insufficient for industrial application. Meanwhile, realistic process design through computer simulation can provide valuable guidance for effective catalyst development.

Key results.

1. Catalyst Screening and Kinetic Modeling

* Corresponding author: Email address:

A screening of potential ETB catalysts for industrial implementation was conducted, resulting in a shortlist of promising candidates. Thermodynamic analysis, compared with experimental data, revealed that the complex ETB reaction network is governed primarily by kinetic factors [1, 2]. Therefore, kinetic modeling is essential for reliable process design and economic evaluation. Simulations show that the two-stage process is superior due to reduced by-product formation. For bifunctional Lebedev catalysts, achieving a balance between dehydrogenation and aldol condensation activity is challenging. Additionally, operating under vacuum conditions and using inert gases improves BD selectivity. Further improvements are needed for getting viable industrial Lebedev catalysts.

2. Technical and Economic Comparison

A comparative analysis was performed for a plant with a capacity of 91,000 tons/year. The two-stage process uses a selective CuO/Cr_2O_3 catalyst for ethanol dehydrogenation and a high-yield Ta_2O_5 catalyst for butadiene synthesis [3]. The one-stage process employs a Hf(IV)/Zn(II) catalyst at an ethanol molar fraction of 0.2 [4]. Simulations were carried out using Aspen Plus™, incorporating kinetic models for reaction systems and systematic methods for flowsheet development and energy integration [7]. The two-stage process demonstrated superior performance, with a BD carbon yield of 83.4%, specific consumption of 0.495 kg-BD/kg-ethanol, and thermal energy use of 16 MJ/kg-BD. In contrast, the one-stage process suffers from lower BD yield and higher costs due to inert gas compression and recycling. Assuming a hypothetical Lebedev catalyst with improved yield and an ethanol molar fraction of 0.5, capital expenditure would increase by 8%, and utility costs by 47%. The best-performing one-stage catalyst ($Ag/ZrO_2/SiO_2$) achieves a BD yield of 73.6%, still below the two-stage process.

3. Fixed-Bed Catalyst Efficiency

Evaluating fixed-bed ETB catalysts requires calculating the efficiency factor. A generic MATLAB method was proposed that can handle multiple reaction schemes involving parallel/consecutive reactions, tackled so far only by sophisticated numerical methods [5]. For one-stage process using kinetic modelling [6] this showed a complex pattern. The method enabled the identification of an optimal catalyst size of 3 mm.

4. Fluidized Bed Reactor Design

Fluidized bed reactors (FB) are suited for ETB processes due to their ability to handle catalyst regeneration. Two-phase kinetic modeling indicates similar performance in the “bubble regime” between mixed-flow and plug-flow patterns by moderate ethanol conversion [1]. This finding simplifies FB reactor design.

5. Energy-Saving via Ethanol Oxy-Dehydrogenation (ODH)

A major breakthrough in energy efficiency can be achieved by applying ethanol oxy-dehydrogenation (ODH) for acetaldehyde production. This reaction releases a significant amount of energy (−173.2 kJ/mol), which can be harnessed for

separation processes and supports autothermal operation. Three alternatives are explored: air oxidation, chemical looping air separation (CLAS) with CuO catalyst, and chemical looping oxidation (CLOX) with Ag/perovskite catalyst. Additional benefits include a temperature drop of over 100°C, near-complete selectivity, high catalyst robustness, and the potential use of CO_2 as an oxidizing agent. This approach is currently at work.

6. Bridging Catalyst Research and Industrial Application

Leveraging systematic conceptual design methods from process systems engineering, along with advanced simulation tools, enables effective investigation of sustainable chemical processes. This integrated approach helps bridge the gap between laboratory-scale catalyst research and industrial implementation.

References:

[1] Dimian, A.C., Bozga, G., Banu, I. Linking catalyst development and chemical reactor design with ethanol to butadiene processes. *MDPI Processes*, 13(4), 1024, 2025.
[2] Banu, I.; Brosteanu, A.-V., Bumbac, G., Bozga, G. Ethanol Conversion to Butadiene: A Thermodynamic Analysis. *Ind. Eng. Chem. Res.*, 2021, *60*, 13071-13083.
[3] Dimian A.C., Bezedea, N.I., Bildea, C.S. Novel two-stage process for manufacturing butadiene from ethanol. *Ind. Eng Chem. Res*., 60 (23), 8475-8492, 2021.
[4] Dimian, A.C., Bildea C.S. Novel one-stage process for manufacturing butadiene from ethanol. Chemical Engineering Research & Design, 193, 460-478, 2023.
[5] Bozga, G., Brosteanu, A.V., Banu, I., Dimian A.C. One-stage ethanol to butadiene process: Analysis and design of a multi-tubular fixed bed reactor. Chemical Engineering Research & Design, 203, 608-618, 2024.
[6] Brosteanu, A.-V., Bozga, G., Banu, I. A kinetic model for the direct conversion of ethanol to 1,3-butadiene. *Univ. Politeh. Buchar. Bull. Ser. B-Chem. Mater. Sci.* 2022, *84*, 112-122.
[7] Dimian A.C., Bildea C.S., Kiss, A.A. Integrated Design and Simulation of Chemical Processes. CACE Series, 35. Elsevier, 2014.

Curriculum Vitae Professor PhD Eng. Alexandre Corneliu Dimian

Professor Alexandre C. DIMIAN obtained the title of engineer at the Faculty of Industrial Chemistry of Politehnica University of Bucharest (UPB) in 1966 and the title of Doctor in Chemical Engineering in 1977. Between 1967 and 1982 he worked in the Chemical Reactors team, in the field of design through mathematical modeling and simulation, but also through experimental investigation.

Since 1882, Professor Dimian began an industrial career in France as a consultant in Computer-Aided Process Engineering (CAPE).

Thus, he had the opportunity to use the most advanced computer systems and CAPE software, which he later applied in his academic work.

In 1993 Alexandre Dimian became a Professor at the University of Amsterdam (UvA) through a competition where he worked until his retirement in 2008. Here he asserted himself as one of the pioneers in Europe in the new discipline of Process Systems Engineering. He supervised doctoral theses including 3 PhDs from

Romania. He is the co-author of numerous publications in top journals in the field, as well as the main author of four books with a worldwide audience published by Elsevier and Wiley.
After 1990, Prof. Dimian returned to Romania to contribute to the modernization of education in Chemical Engineering. He participated in the actions to improve university education, including the implementation of a CAPE center at UPB. Prof. Dimian has biographical notes in "Who's Who in the World" and "Who's Who in Science and Technology", is awarded the DHC at UPB and a he is member of the Romanian Academy of Technical Sciences. Today, Professor Dimian carries out sustained activity in the field of the design of sustainable chemical processes based on renewable resources. The scientific performance can be assessed through www.scholar.google.ro (September 2025): 4450 citations, H-index 30, approx. 22000 readings/year

PL02 NOVEL NANOMEDICINE FROM NATURE: A SUSTAINABLE GREEN APPROACH

Sougata Ghosh*

Department of Microbiology, School of Science, RK. University, Rajkot, Gujarat, India

Abstract: *Nanomaterials with shape and size-dependent physicochemical and optoelectronic properties can be designed using several physical and chemical methods. However, hazardous reaction conditions and toxic chemical reagents used in these methods compromise the biocompatibility of the synthesized nanoparticles, making them unsuitable for biomedical applications. Hence, several environmentally benign biological routes have been designed to synthesize gold, silver, platinum, palladium, copper, and bimetallic nanoparticles using viruses, bacteria, fungi, algae, and medicinal plants. As a part of our growing interest in the novel nanomedicine, we have developed methods to use various medicinal plants found in nature, like Dioscorea bulbifera, Gnidia glauca, Plumbago zeylanica, Barleria prionitis, Gloriosa superba, and many more, for synthesizing nanospheres, nanohexagons, nanotriangles, and nanorods. Careful optimization of time, temperature, pH, and concentration of metal salts may help in the synthesis of nanomaterials with well-defined shape and size. Further, naturally occurring bioactive principles like curcumin, diosgenin, etc., may stabilize and enhance the anticancer, antioxidant, antidiabetic, antimicrobial, and antibiofilm activities of the biogenic nanoparticles. In view of the background, it can be concluded that there is a huge scope for further research towards the translation of the biogenic nanoparticles as potential nanomedicine in the future*.

Keywords: Nanoparticles, biological synthesis, medicinal plants, functionalization, biomedical applications.

BRIEF BIOGRAPHY Dr. Sougata Ghosh

1) Dr. Sougata Ghosh is currently working as an Associate Professor in the Department of Microbiology, School of Science, RK University, Rajkot, Gujarat. He is also a Visiting Professor at the Department of Physics, Faculty of Science, Kasetsart University, Bangkok, Thailand. He is an active researcher in nanomedicine, who obtained his Bachelor's degree, Master's, and Ph.D. in Microbiology from the University of Pune, presently Savitribai Phule Pune University, India. He was a Postdoctoral Fellow at **Northeastern University, USA.**

2) **He has filed 8 patents, 271 publications that include 10 Books, 168 book chapters, and 93 international research and review articles.**

* Corresponding author: ghoshsibb@gmail.com
Dr. Sougata Ghosh Ph.D. (India), Post Doc. (USA; Thailand)
Associate Professor, Department of Microbiology, School of Science, RK. University,
Rajkot, Gujarat, India.
Contact: +91-9923268332.

3) He has **6062 citations, h-index 42,** and **i10-index 104. He is listed among the World's Top 2% Scientists for 2025, 2024, 2023, and 2022, as released by Stanford University, USA, and Elsevier.** He has published in highly cited international journals, including the International Journal of Nanomedicine, Journal of Nanobiotechnology, Journal of Nanomaterials, and Journal of Nanoscience and Nanotechnology.

4) He has served as resource person and invited speaker in **160 international and national conferences, symposia, and workshops** the most notable being ICMAR 2023 at Cebu Normal University, **Philippines**; 1st JICEST-2023 at University of Jambi, **Indonesia**; IMRC-2022, **Mexico**; IJAS-2019 at **Harvard University**, **USA**; ASM Biodefense, Washington D.C. **USA**; Nano-Bio-Med 2013, **Italy** and BioMicroWorld2013, **Spain**.

5) Dr. Ghosh is **Associate Editor of Frontiers in Chemistry, Current Microbiology (Springer),** and also a member of the **Editorial Board/Reviewer's Team** of **101 international journals** like Nanoscale, Journal of Photochemistry & Photobiology, B: Biology, Journal of Diabetes Research, International Journal of Advances in Engineering Research, and others.

6) He was Principal Investigator of **DBT (Department of Biotechnology),** Government of India, funded the Foldscope Project, and had conducted numerous workshops in various Colleges and Universities throughout India, where more than 1200 students received training on research and innovation using Foldscope.

7) He has received several prestigious awards, like

i) Junior Research Fellowship (JRF)-2011 by Institute of Bioinformatics and Biotechnology (IBB), University of Pune, Pune, India.
ii) Senior Research Fellowship (SRF)-2012 by Council of Scientific and Industrial Research (CSIR), Government of India, New Delhi.
iii) DST-Overseas Visiting Fellowship-2019 in Nanoscience and Technology by Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India.
iv) Reinventing University Program Fellowship-2021/22 by Kasetsart University, Bangkok, Thailand.
v) Bharat Gaurav Puraskar – 2024 by KTK Outstanding Achievers and Education Foundation, New Delhi, India, for outstanding achievements and remarkable contribution in the field of Microbiology.

.

PL03 PROCESS MODELLING THROUGH ANALOGIES: CUSTOMIZE FOR MODELLING OF BLOOD DIALYSIS BY ANALOGY WITH A HEAT TRANSFER CASE

T. Dobre[1, 2, *]

[1]National University of Science and Technology Politehnica Bucharest, Chemical and Biochemical Engineering Department, 1-7 Gheorghe Polizu St., 011061 Bucharest, Romania, [2]Technical Sciences Academy of Romania, 26 Dacia Boulevard, 030167, Bucharest, Romania

Abstract: *The use of analogies in process modeling has been and will be a successful solution. We exemplify this with a heat transfer-mass transfer analogy applied to blood dialysis modeling.*
Key words: Transfer analogies, Dialysis, Hemodialysis, Coil heating model, Mathematical modeling, Peritoneal hemodialysis simulation

Introduction: The Reynolds, Prandtl-Taylor and von Karman analogies [1], based on the similarity of the hydrodynamic thermal and diffusion boundary layers explain well the criterial relationships used in heat and mass transfer [1]. Here is considered the analogy between the cooling of a warm liquid flowing through a coil in a perfectly mixed cold liquid [1] and the membrane blood dialysis with a perfectly mixed dialysis medium [2].

Modelling and results: Specifically, here the mathematical model of heating through the coils of a perfectly mixed liquid is particularized to the case of blood dialysis in hallow fiber membrane with perfectly mixed dialysate. First simulation cases consider the species, urea and respectively creatinine, transfer from blood to a fixed dialysate volume through a tubular hollow fiber's membrane with a fixed mass transfer area. This hemodialysis case corresponds, for the most part, to peritoneal hemodialysis [3]. It shows what are the factors and parameters that must be considered in this case and brings simulation cases related to cyclic peritoneal hemodialysis [4]. Our model is new relative to ones overviews of computational models on peritoneal dialysis (PD). All general and individual aspects of the PD models aim to simplify, enhance, and accelerate the integration of modeling into clinical practice to promote better understanding of device-patient interaction. Our paper temptation can be considered in the sense not only bydeveloping a new PDmathematical model near to other existing in this problem.

References:

[1] Bratu Em., *Unit Operations in Chemical Engineering, Kastkin Problem*, Vol. 2, Technical House, Bucharest, 1983.
[2] Thews O., Hutten H.A comprehensive model of the dynamic exchanges during hemodialysis,*Med. Progr. Technol*.1990, 16, 145-161,
[3] Walther L.J., Bartlett W.D., Chew W., Robertson R.C., Meyer W.T., Downloadable computer models for renal replacement therapy, *Kidney International.* 2006, 69, 1056–1063.

* Corresponding author: tghdobre@gmail.com

[4] SwapnasritaS., Joost C de Vries C.J., Oberg M.C., Carlier M.F. Aurelie, Gerritsen G.F. Karin,Computational modeling of peritoneal dialysis: An overview,*Math. Biosci. Eng.* 202522, 2, 431–476.

About the author: Tanase G. Dobre, graduates from Bucharest Politehnica University in Industrial Chemistry and Processes Engineering, begins as engineer by working in production, design and research in Printed Boards Technology, at the factory Felix Computers Bucharest. He gains, at Bucharest Politehnica University, a Chemical Engineering Assistant position starting like his university activity, The topic of his PhD thesis was in modelling and experimental investigation of the wetted mobile packed bed as a basic structure in heat and mass transfer enhancement. He was strongly involved with the modelling and experimental investigation aspects concerning the transposition to the industrial scale of the process concerning the sulphur separation from the flotation suspensions. He was a member of a national consortium with a research object in the field of heat pipes where he insisted, experimentally and through modelling, for their use in temperature control in chemical reactors.On the way of his university promotion, he kept in the foreground transfer phenomena and modelling and simulation of processes, for research and equipment design. About six years he is in a strongly cooperation with ENSCh Montpellier with works in membrane processes modelling and simulation. His main research interest covers mathematical modeling and computer simulation of chemical and biochemical processes, stochastic processes, mass transfer with porous medium (membrane processes), mathematical modeling of air, soil and water pollution, intensive processes by heat and mass transfer enhancement, advances in separation processes computing, simulation, and experimental checking. He is a member of the Technical Sciences Academy of Romania and of Romanian Chemical Engineering Society, which he represents nationally and internationally, especially at the European Federation of Chemical Engineering.

PL04 CURRENT AND FUTURE APPLICATIONS OF MESOPOROUS SILICA

Dan-Adrian Vasile[1-3], Gabriela Petrisor[1-4], Mariana Jian[1,5], Rucsandra Dumitrescu[1-3], Ludmila Motelica[1-5], Natalia Dragut[1], Angela Spoiala[1-3,5], Roxana Trusca[2,3], Ovidiu Oprea[1-4], Dan Mihaiescu[1-3], Coralia Bleotu[4,5], Denisa Ficai[1-4], Viorel Nacu[5,6], Anton Ficai[1-4, *]

[1]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania
[2]National Center for Micro and Nanomaterials, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania,
[3]Research Center for Advanced Materials, Products and Processes, National University of Science and Technology Politehnica Bucharest, 060042, Bucharest, Romania,
[4]Academy of Romanian Scientist, Bucharest, Romania
[5.] Laboratory of Tissue Engineering and Cell Cultures, Nicolae Testemitanu State University of Medicine and Pharmacy, Stefan cel Mare street 165, Chisinau, Moldova
[6] Human Cells and Tissue Bank, Traumatology and Orthopedy Clinic Hospital, Stefan cel Mare street, 190, Chisinau, Moldova

Abstract: *The history of the mesoporous silica started in 1992 and, during the ~3 decades of intensive research and development many synthesis and modification techniques were developed and consequently new applications were identified, in various field such as medicine, energy or environmental protection. The presentation, is mainly focused our recent advances in the field of synthesis of these mesoporous materials via the classical sol-gel route and their chemical modification. The use of greener synthesis routes will be also presented, being in line with the actual EU trends by using starch instead of the classical CTAB. Regardless the synthesis, these mesoporous materials were loaded with a wide range of agents in order to develop materials with potential applications in: the treatment of dysbiosis, food supplements, drug delivery systems, latent fingerprint development, environmental applications, especially pollutants removal; etc. For all these applications a special attention will be paid to the materials design, including the synthesis itself, the chemical surface modification and loading of the proper active agents (dyes, polyphenols, antibiotics, natural oils/extracts, etc.).*

[*] Corresponding author: anton.ficai@upb.ro
viorel.nacu@usmf.md

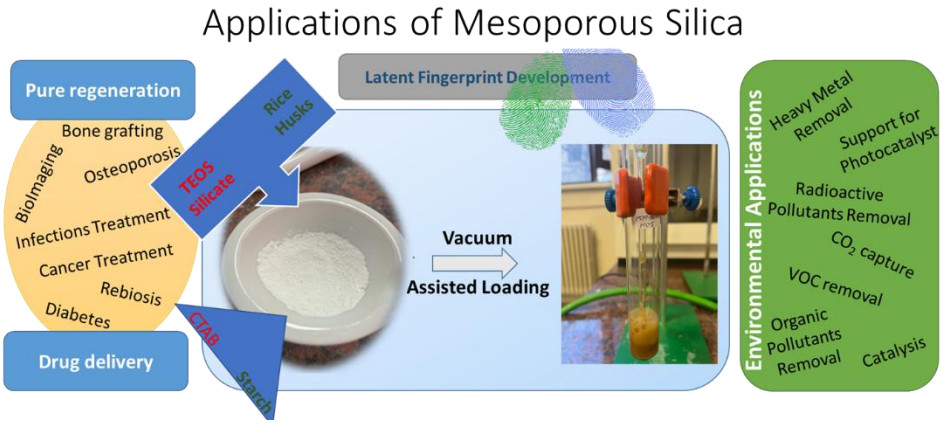


Figure 1. Current and Future Applications of Mesoporous Silica

Key words: Mesoporous Silica; Surface Chemistry; Medical and Non-medical Applications
Acknowledgments: The authors are acknowledging the support of the project 29ROMD/20.05.2024: "Nanostructured bone grafts with predetermined properties".

Short Biography

Anton FICAI (born 1981) is full professor and PhD advisor in the Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology POLITEHNICA Bucharest being actively involved in both academic and scientific life of the university. His major academic interests are related to Composite Materials for Medicine, NanoBioMaterials for Tissue Engineering and Drug Delivery Systems. The research interests are much broader, having the chemical approaches in the center, and cover the following topics: tissue engineering; drug delivery systems; multifunctional materials; composite materials; coatings, antimicrobial / antitumoral materials; nanoparticles synthesis and characterization; surface modification; etc. Till now, over 370 scientific papers, from which over 330 ISI papers and 24 books or chapters (including 3 edited books) were published along with 28 patent applications (10 of them being already released). The international recognition of the R&D activity can be highlighted by the multiple invitations for participate as speaker at international conferences, the positions of guest editors, member of the editorial boards of different national and international journals as well as Section Editor in Chief of Coatings. Valedictorian of UPB, former participant and laureate of the National Chemistry Olympiads he was awarded with over 150 Gold Medals, Special Awards or Best Paper Awards and recently, he was awarded with the Special Award for Transfer of the Research Results into Economy by the Ministry of Resort during the First edition of the "Gala Cercetării Românești". He is also full member of The Academy of Romanian Scientists and several professional societies.

PL05 PROCESS INTENSIFICATION APPLIED FOR EXTRACTION OF NATURAL PRODUCTS

Ioan Călinescu*, Mircea Vinatoru

NUST POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, Bioresources and Polymer Science Department, 1-7 Gh. Polizu str., 011061, Bucharest, Romania

Abstract: *With growing consumer demand for natural products, greener extraction techniques are found to be potential alternatives, especially for pharmaceutical, nutraceutical, and cosmetic manufacturing industries. This review includes a detailed overview of the ultrasound-assisted extraction (UAE), microwave-assisted extraction (MAE), and combined extraction techniques, which have been implemented for the extraction of high-value-added compounds.*
The main types of equipment that can be used for assisted extraction are presented, mentioning the advantages and limitations of each type of equipment. A list of essential parameters necessary for the maximum possible extraction yield has been discussed for each method. The experimental results confirm the principles of intensification of extraction processes with these techniques.

Introduction: Extraction of numerous products and their applications has been prevalent since ancient times. Extraction is an essential part of the production line in food, cosmetic, pharmaceutical, and nutraceutical industries, and hence the advancement in extraction technology will bring significant benefits in terms of energy consumption, pollution abatement, as well as producing a better quality of extract.

Although many types of techniques and equipment can be used to intensify extraction processes, their use is not always done appropriately. There is often a risk of degradation of the active ingredients to be obtained or the realization of extractions with low selectivity, in which, in addition to the target product, there are many other by or undesired compounds.

Ultrasound-assisted extraction (UAE) and microwave-assisted extraction (MWE) are novel, greener extraction alternatives employed in recent years.

Objectives : The paper presents several types of equipment with numerous uses (multimode microwave applicator, ultrasonic bath), suitable for extraction of natural compounds, but which are not always described and effectively used. For these equipment, specific characteristics operations and procedures that allow obtaining reliable and valuable results are presented. Less known types of equipment are also presented, for example, a "coaxial antenna and a cooling system" for intensifying microwave processes or a "dual-frequency reactor" for the use of ultrasound. A special chapter is also dedicated to original equipment for the simultaneous use of ultrasound and microwaves.

* Corresponding author: ioan.calinescu@upb.ro, Tel.+40745371285

Materials and methods: For each type of equipment, experimental data are presented that allows a better understanding of the working procedures that enable efficient natural product extraction processes :

- Evaluation of the maximum amount of desirable compound that can be extracted by multiple successive extractions [1] ;
- Modeling the temperature field dynamics during microwave-assisted extraction [2];
- Selective and volumetric heating during microwave extraction [3];
- Microwave-assisted extraction using a coaxial antenna and a cooling system [4];
- Mapping an ultrasonic tank for sonochemistry [5];
- Use of a US dual-frequency type reactor [6]
- Combined use of microwave and ultrasound to intensify extraction processes [7-9]

Conclusions: Intensifying natural extraction substances processes is an effective method to achieve "green extraction". Microwaves and ultrasound are two effective methods for intensifying processes. Although there is a multitude of laboratory equipment that can be used in this regard, the right choice of working parameters is essential for optimizing the extraction process. Although general principles can be formulated for the selection of these extraction conditions, it should be noted that they could be different for each type of substrate and for each target compound.

References:

1. Gavrila, A.I., Zalaru, C.M., Tatia, R., Seciu-Grama, A.M., Negrea, C.L., Calinescu, I., Chipurici, P., Trifan, A., and Popa, I., "Green Extraction Techniques of Phytochemicals from Hedera helix L. and In Vitro Characterization of the Extracts", *Plants-Basel*, **2023**. *12*(22): p. 17, https://doi.org/10.3390/plants12223908.
2. Lavric, V. and Calinescu, I., "Modeling the Temperature Field Dynamics During the Microwaves Assisted Extraction of Active Principles from Vegetables". in Proceedings of the 16th International Conference on Microwave and High Frequency Heating (AMPERE), Delft, The Netherlands. **2017**.
3. Galan, A.M., Calinescu, J., Trifan, A., Winkworth-Smith, C., Calvo-Carrascal, M., Dodds, C., and Binner, E., "New insights into the role of selective and volumetric heating during microwave extraction: Investigation of the extraction of polyphenolic compounds from sea buckthorn leaves using microwave-assisted extraction and conventional solvent extraction", *Chemical Engineering and Processing*, **2017**. *116*: p. 29-39, https://doi.org/10.1016/j.cep.2017.03.006.
4. Calinescu, I., Lavric, V., Asofiei, I., Gavrila, A.I., Trifan, A., Ighigeanu, D., Martin, D., and Matei, C., "Microwave assisted extraction of polyphenols using a coaxial antenna and a cooling system", *Chemical Engineering and Processing: Process Intensification*, **2017**. *122*: p. 373-379, https://doi.org/10.1016/j.cep.2017.02.003.
5. Mason, T.J., Ghimpeteanu, D., Călinescu, I., Vinatoru, M., and Trifan, A., "A simple new approach for mapping an ultrasonic tank for sonochemistry", *Ultrasonics Sonochemistry*, **2024**. *107*: p. 106940, https://doi.org/10.1016/j.ultsonch.2024.106940.
6. Quaratesi, I., Calinescu, I., Lavric, V., Ferrara, V., Badea, E., Chipurici, P., Dumbrava, E.-G., Constantinescu, R.-R., Ignat, N., and Popa, I., "Loop-Ultrasound-Assisted Extraction:

An Efficient Approach for the Recovery of Bioactive Compounds from Oak Bark", *Agronomy*, **2024**(14), https://doi.org/10.3390/agronomy14071452.

7. Vinatoru, M. and Calinescu, I., "Microwave and Ultrasounds together - a challenge". in 17th International Conference on Microwave and High Frequency Heating (AMPERE). **2019**. Univ Politecnica Valencia, Polytechn City Innovat, Valencia, SPAIN: Univ Politecnica Valencia, https://doi.org/10.4995/Ampere2019.2019.9822.
8. Vinatoru, M., Mason, T.J., and Calinescu, I., "Ultrasonically assisted extraction (UAE) and microwave assisted extraction (MAE) of functional compounds from plant materials", *TrAC Trends in Analytical Chemistry*, **2017**. *97*: p. 159-178, https://doi.org/10.1016/j.trac.2017.09.002.
9. Călinescu, I., Vinatoru, M., Ghimpețeanu, D., Lavric, V., and Mason, T.J., "A new reactor for process intensification involving the simultaneous application of adjustable ultrasound and microwave radiation", *Ultrasonics Sonochemistry*, **2021**. *77*: p. 105701, https://doi.org/10.1016/j.ultsonch.2021.105701.

(https://eertis.eu/errf-2300-000c-2090)

Prof. Ioan Calinescu received his chemical engineering education (M.Sc. and Ph.D.) from the University POLITEHNICA of Bucharest. His research interest includes the use of microwave, electron beam, and ultrasound in intensifying processes related to biomass processing and biofuels production, as well as removing various pollutants from the gaseous or liquid media. He co-authored over 125 peer-reviewed papers and 11 patents in these areas. He is a doctoral supervisor with 27 PhD students who supported his doctoral thesis under his guidance. He has been responsible for more than 20 national and international projects, of these 3 projects had as their object of research the extraction of active ingredients from plants. He is the coordinator of a research platform dedicated to the use of ultrasound and microwaves in process intensification

PL06 MODULAR NUCLEAR POWER PLANT DOICESTI PROJECT

Serban Constantinescu

Introduction: The latest technology of small nuclear reactors for power is close to be implemented in Romania, thanks to a good co-operation between the US and Romanian governments.

US Nuscale has developed, tested and verified this new technology, all parameters, certifications being approved by all American and International entities, and we are excited to be the first foreign partner to implement this.

However, the positioning of this new power plant in Doicesti, a village situated about 80 km north of Bucharest, next to a small river, has raised a few questions in my mind, even if I am far from being a nuclear engineer.

The presentation below will analyze, briefly, some aspects, such as seismicity, water supply, exclusion and restricted areas, connection to the national grid network and operating specialists training.

As a general idea, nuclear technology for power plants has some specific aspects, different to the classic ones on coal / lignite / gas power plants and choosing the right place for such plant is not an easy task for any project manager.

For sure, a business plan will follow soon, all aspects of the positioning will have a big effect in costs, time and energy spent; at the end, the result of each KW or MW produced should be competitive and at the market level, to have arguments for immediate approvals and start-up of the construction.

With this new project, we want to have:

- continuous power supply in our national system
- people and environment security
- green energy
- competitive production prices
- a reference project for other such businesses

PL07 ANALYSIS OF THE SILICATE AND OXIDE COMPOUNDS INDUSTRY

Doru Vladimir Pușcașu, Maria Georgescu

Technical Sciences Academy of Romania, 26 Dacia Bld, 030167, Bucharest, Romania

Abstract: This scientific paper is intended to be an up-to-date overview of the situation of manufacturers of the silicate and oxide compounds industry: ceramics (household and ornamental ceramics, sanitary ceramics, ceramic tiles and slabs, ceramic bricks and tiles, refractory ceramics), binders (cement, lime, plaster and concrete) and glass (flat glass, flat glass processing and shaping, manufacture of glass articles, manufacture of glass fibers). The economic data for each sector of activity (number of companies, turnover, profit, number of employees, and profit/employee ratio in 2024, based on balance sheet data) are presented, as well as the evolution of these economic indicators over the last five years. Also based on data from 2024, the top five companies in each activity are presented, according to their turnover. A SWOT analysis is then performed for each sub-sector, highlighting strengths, weaknesses, opportunities, and threats. The conclusion of the paper presents the overall situation of manufacturers of binders, ceramics, and glass.

Key words: cement, concrete, ceramics, glass

Dr. Eng. **Doru Vladimir Pușcașu**, first degree scientific researcher, has worked for over 50 years at the CEPROCIM S.A. Research Institute in Bucharest, going through all the hierarchical levels, from trainee engineer to Team Leader, Section Head, Scientific Director, General Manager and President of the Board of Directors.

In his activity, he participated in the research and studies that formed the basis for the construction of all cement factories in Romania after 1971 (Aleșd, Tg.Jiu, Câmpulung, Medgidia, Fieni, Deva, Hoghiz, Tașca-Bicaz) as well as in the technological studies necessary for the design of cement factories exported by Romania to Yugoslavia/Croatia/Bosnia and Herzegovina, Syria, Egypt, Lebanon, Pakistan, China, Iran, Philippines. He participated in the commissioning and demonstration of the designed parameters of the 800 t clinker/day lines from Aleșd, Tg.Jiu, Câmpulung, Fieni, and the 3000 t cl/day ones from Hoghiz, Deva, Tașca, Aleșd, Medgidia. He also participated in the commissioning and demonstration of the guaranteed parameters of the cement manufacturing line from Koromačno (former Yugoslavia) exported by Romania, as well as in the implementation of modernization activities or the creation of new products at the cement factories Devnia (Bulgaria), Sheikh-Said (Syria), Askale (Turkey), Našice (Croatia).

His professional activity has resulted in participation in the implementation of research projects from the National Research and Development Plans of Romania, as well as direct contracts with economic agents. He has participated as project director/theme manager in the implementation of over 350 research themes. He was the main author/co-author/or author of chapters in six books or chapters of specialized books and is the author of three patents.

Since 2012 he has been a corresponding member of ASTR and since 2020 a full member. He was Scientific Secretary of Section 8 – Chemical Engineering, and since 2020 President of the Section.

***

Professor **Maria Georgescu** has worked as a teacher for over 50 years at University POLITEHNICA of Bucharest, contributing to the training of numerous engineers in the field of Chemistry and Technology of Silicates and Oxide Compounds. In parallel with her teaching activity, she has carried out a sustained scientific research activity, with a varied theme, in the specialized field, such as: processes in the formation of Portland clinker and in the hardening of cement, complex binders with hardening through hydration-hydrolysis reactions, complex binders with hardening through hydration-hydrolysis reactions or acid-base reactions, additions and additives in complex binder systems, synthesis of binders through unconventional methods, valorization of waste in obtaining binders.

The results of scientific research have resulted in over 240 scientific papers published in specialized journals in the country and abroad, or communicated at national or international scientific events. She has developed, in collaboration, 12 books in the field of chemistry and technology of binders or related fields, useful materials in the training of students, as well as updating the specialized knowledge of graduates, necessary in practical activities.

Doctoral supervisor, Mrs. Prof. Maria Georgescu, guided the activity of improving graduates through this form of education between 1991 and 2012, for a number of 17 graduates who completed and defended theses well appreciated by specialists in the field. Since 2012, she has been a full member and works within the Romanian Academy of Technical Sciences, Chemical Engineering section..

PL08 PRESSING CHALLENGES IN OIL REFINING INDUSTRY

Claudia I. Muntean[1]

[1] Ovidius University of Constanta, 124 Mamaia Blvd., Constanta, 900527, Romania

Abstract: *This presentation deals with the rapid transformations in front of the oil processing industry, some of them unexpected a few years ago: the new global energetic strategy, the change in extracted oil quality, the market dynamic, the environmental regulations, the technical challenges, and more than others, the operational constraints. The industry continuously seeks solutions; some are in the process of adapting but others are still expected to be discovered.*
Key words: oil refining industry, strategic challenges, new technologies, environmental regulations, operational challenges

Introduction: The petroleum refining industry has a respectable history of 150 years, during which it has had many accomplishments. It was the main fuels provider for transportation, home heating, agriculture, and industry; it is the primary raw material supplier for petrochemical industry and the main solvents supplier. For decades, the progress of technologies and management felt comfortable in the petroleum refining industry. This situation is no longer valid with the challenges urging in the present.

Pressing challenges in oil processing industry:

- The new strategic challenges- the energy landscape shifting towards renewable resources, the target of 80% alternative energy by 2030 used to be a long- term challenge; the remaining time now makes this target questionable, but the effects on the petroleum industry are strongly felt. Increasing cyberattacks -the other strategic challenge- poses an urgent need to protect the infrastructure.
- The change in extracted oil quality is due to less exploration of new deep reservoirs and the increasing use of shale oil, an unconventional raw for refineries; by processing heavier and worse quality oil, this leads to lower yields of white products, increasing processing costs, and more problems with corrosion and waste management.
- Market dynamics and economic challenges -the price volatility of crude and products makes the financial planning risky and impacts the profitability of the company; the company profit margins are also affected by the rising costs with the exploration, production, investment, labor; the complexity of the supply chain can lead to disruptions in any point such as upstream operations, transportation, equipment failure, materials supply, etc.
- Environmental regulations- pressure of public and institutions to mitigate the carbon footprint of this industry causing climate changes, and to reduce the pollutant emissions in air, soil and water, have resulted in strict regulations whose implementation demands massive investment in clean technologies and operational changes.
- Technology challenges- new generation catalysts with improved activity and selectivity are required to ensure superior yields and products quality; more efficient separation processes are required for the same purpose; the integration of petroleum refining with the petrochemical processes and possibly with lubricant

facilities was demonstrated to add value to the crude oil. All measures responding to the technological challenges have as a final goal profitability increasing and compliance with environmental requirements.

- Operational constraints: tank limitations (available storage capacity, limited flexibility, minimum residence time), pipe limitations (connectivity to units); maintenance scheduling complexity, aging infrastructure; complexity of operations needing digital transformation; highly qualified workforce, difficult to attract and retain.

Conclusions: All the challenges mentioned above require careful examination and solutions. For some, the experience and time to solve them is enough, but some emerge suddenly and there are situations where the industry is off-guard. Continuous information and communication across stakeholders are essential to prevent the occurrence of blockages.

References:

[1] Shah, N.K., Li, Z., Ierapetritou, M., Petroleum Refining Operations: Key Issues, Advances, and Opportunities, *Ind. Eng. Chem. Res.*, 50 (2011), 1161–1170
[2] Degnan, Th., Chemical reaction engineering challenges in the refining and petrochemical industries - The decade ahead, *Curr. Opin. Chem.Eng*., 9 (2015), 75-82
[3] Lima, R.A.O., Guirardelo, R., Long-Term Turnaround Planning for an Oil Refinery using a MILP Model, Chem. Eng. Trans., 117 (2025), 1027-1032

With a degree and a PhD in Chemical Engineering from Oil&Gas University of Ploiești Romania, and with an industrial background, Professor Claudia Irina Muntean (Koncsag) worked for 30 years at Ovidius University of Constanța, Romania, teaching Chemical Engineering subjects and Oil Processing, as her specialization. Professor Muntean also had a long and fruitful research activity. Between 2014-2023, she was the President of Constanța Branch of SICHEM. Since 2022, she is retired but still active in research and in industrial environment as an expert for carbon emissions evaluation and for other commissioning activities.

PL09 PHYCOREMEDIATION OF OLIVE MILL-WASTEWATERS

Bouthaina Menaa[1,3], Rihab Hachicha[1,3], Pascal Dubessay[1], Slim Abdelkafi[2], Imen Fendri[3], Philippe Michaud[1*]

[1] Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, F-63000 Clermont–Ferrand, France., Clermont Auvergne University, 63000 Clermont-Ferrand, France

[2] Laboratory of Plant Biotechnologies Applied to Crop Improvement, Faculty of Sciences of Sfax, University of Sfax, 3038 Sfax, Tunisia

[3] Laboratory of Enzymatic Engineering and Microbiology, Algae Biotechnology Team, National School of Engineers of Sfax, University of Sfax, 3038 Sfax, Tunisia

Abstract: *The olive oil industry generates approximately 30 million m³ of olive mill wastewater (OMWW) annually, posing significant environmental challenges due to its high content of organic matter, suspended solids, dark coloration, and unpleasant odor. This study aimed to optimize the bioconversion of OMWW through physicochemical, enzymatic, and microbial treatments. Primary treatments such as coagulation-flocculation and adsorption were investigated. A hybrid system combining activated carbon and chitosan proved to be the most effective in reducing the pollutant load of these effluents. Enzymatic pre-treatment of OMWW diluted to 30% with fungal laccases significantly reduced phenolic compound concentrations and coloration, making the medium suitable for the mixotrophic cultivation of Chlorella sp. and Tetraselmis sp.*

Although microalgal growth and pigment production under mixotrophic conditions were lower compared to photoautotrophic culture, Chlorella sp. exhibited increased protein synthesis. A comparative analysis of the proteomic and transcriptomic profiles of Chlorella sp. revealed an overexpression of cell cycle-related proteins under mixotrophic conditions. Despite a reduction in photosynthetic activity, chlorophyll production was maintained due to the activity of the DPOR enzyme. The overexpression of acetyl-CoA carboxylase and ammonium transporters suggests a metabolic shift favoring chlorophyll biosynthesis

Keywords: Olive mill wastewaters ; microalgae ; laccases ; bioremediation ; omics

* Corresponding author: philippe.michaud@uca.fr

Brief Bio-sketch

Philippe Michaud, *Full Professor* of biochemistry since 2005, is head of the "4Bio" research group at the Institut Pascal, an interdisciplinary research laboratory of Clermont Auvergne University. Since 2023 he is President of the National Council of Universities for biochemistry and molecular biology.

His scientific skills focus on the development of bioprocesses for obtaining polysaccharides from various sources and analysis of their structure-function relationships. He has published 298 research papers and 22 book chapters. He is the co-inventor of 14 patents, 3 of them leading to industrial exploitation. He has been the advisor or co-advisor for 28 PhD students. Since 2005, he has been in charge of more than 30 national and international research projects, funded or co-funded by industry. He was the general secretary of International Forum on Industrial Bioprocesses between 2015 and 2018. He is topical chief editor of Euro-Mediterranean Journal for Environmental Integration and associate or guest editors of numerous international journals. He has been nominated as *Chevalier des palmes académiques* in 2020 and received a Distinguished Scientist Award for the year 2021-2022 by the International Bioprocessing Association.

PL10 HYDROGEN–WATER INTERFACES: RECENT INSIGHTS AND APPLICATIONS TO ENERGY CONVERSION

Christophe Vial[1,*], Adib Essid[1], Blandine Tauleigne[1], Alina-Violeta Ursu[1], Alain Marcati[1], Jean-Sébastien Guez[1]

[1] Clermont Auvergne Université, Clermont Auvergne INP, CNRS, Institut Pascal, Clermont-Ferrand, F-63000, France

Abstract: *Hydrogen–water interfaces and gas–liquid mass transfer in aqueous media play a pivotal role in hydrogen production, conversion, and storage processes that drive the global energy transition. Key applications of the energy sector, including water electrolysis, (photo)biological hydrogen production, hydrogen fuel cells, biological methanation, and geo-methanation, critically depend on these interfaces. To elucidate their role, hydrogen–water interactions must be investigated at the bubble, bubble swarm, and process scales, under varying temperature, pressure, and aqueous medium compositions relevant to energy applications. Recent studies conducted at Institut Pascal, encompassing three Ph.D. programs, will be used to illustrate the potential and limitations of both conventional and advanced measurement techniques applied at several scales for determining key parameters such as hydrogen solubility, diffusivity in the liquid phase, surface tension, interfacial area, and mass transfer coefficients. These approaches include local probes, high-speed imaging, and artificial intelligence-based analysis. Typical results will be presented and correlated to experimental conditions. Special emphasis will be placed on the challenges of extrapolating oxygen mass transfer data to hydrogen gas and on the consequences of this assumption. Addressing these challenges is essential to develop more efficient and sustainable hydrogen-based technologies. The case of biological methanation within the power-to-gas strategy will be presented as a detailed example.*

Key words: Hydrogen production; power-to-gas; gas-liquid mass transfer; hydrogen solubility.

About the author: Dr. Christophe Vial is a Professor of Chemical Engineering at Clermont Auvergne University in France. He is also the Head of the Energy Master's Program at Polytech Clermont. Since 2017, he has served as the Deputy Director of Institut Pascal, an interdisciplinary engineering research unit with 400 members. His research focuses on hydrodynamics and mass transfer in gas–liquid and gas–liquid–solid bubbly flows, with applications in bioenergy, food, chemical, and environmental engineering. He has co-authored 140 research papers and about 220 conference and seminar communications on these topics. Dr. Vial has supervised or co-supervised 25 Ph.D. students (including 5 ongoing), among them 6 in international joint Ph.D. programs. In 2024, he co-founded a startup company dedicated to biological methanation for biogas upgrading from anaerobic digesters.

* Corresponding author:

PL11 TOWARD HYBRID PHOTOREACTIVE SYSTEMS FOR ENERGY AND ENVIRONMENTAL APPLICATIONS

Fabrice Gros[1,*], Jérémi Dauchet[1], Thomas Vourc'h[1], Jean-François Cornet[1]

[1] Clermont Auvergne Université, Clermont Auvergne INP, CNRS, Institut Pascal, Clermont-Ferrand, F-63000, France

Abstract: *Photoreactive systems have emerged as promising tools for sustainable energy and environmental technologies. Building on our previous contributions, this work proposes an integrated methodology for the conception, modelling and experimental validation of hybrid photoreactive processes coupling solar-driven reactions and chemical engineering approaches.*
Our general framework hence combines: the radiative and thermokinetic modelling of the processes, from the catalyst optical properties to the full 3D light distribution; experimental design and validation, using tailored photoreactors and spectro-radiometric measurements; hybridization strategies, where photo-assisted processes are coupled with classical operations such as airlift or photovoltaic conversion.
The latest advances in the study of photoreactive processes will also be presented. Several examples will be discussed, from photocatalytic hydrogen production to photo-assisted depollution of aqueous media, highlighting the predictive capability of the proposed multiscale model and its potential for process intensification and reactor design optimization.
Key words: Photoreactive process, Hybrid systems, Solar fuels, Modelling.

About the author: Fabrice GROS is full professor at Sigma Clermont since 2018. He is engineer in chemical engineering of the Grenoble INP, where he also obtained a PhD Thesis in electrochemical process engineering in 2005. He obtained in 2017 an HDR at the Clermont Auvergne University in his current research domains in the study and the modeling of photoreactive processes and their three main applications: photobioreactor, photoreactor, photoelectrochemical cell. He is now the director of studies in SIGMA Clermont. He was also head of the Chemical Engineering Department at Sigma Clermont from 2018 till 2021 and deputy manager of the axe GePEB of the Pascal Institute from 2017 till 2023. He is also member of the board of the Société Française de Génie des Procédés, and president of Comité de Développement du Génie des Procédés en Région Rhône Alpes Auvergne (Codegepra). He is the project leader for the organisation of the 20th congress of Société Française de Génie des Procédés in 2026 in Clermont-Ferrand.

PL12 IMMOBILIZED ENZYME MONOLITHIC PLATFORM FOR FUNCTIONALIZING POLY- AND OLIGOSACCHARIDES

Xiaoyang Hou[1], Gwendoline Christophe[1], Philippe Michaud[1], Pascal Dubessay[1], Guillaume Pierre[1,2,*]

[1] Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, F-63000 Clermont-Ferrand, France

[2] Institut Universitaire de France (IUF), 1 rue Descartes, 75005 Paris, France

Abstract: *The exploitation of functional poly- and oligosaccharides has attracted extensive interest due to their diverse applications in cosmetics, health, nutraceuticals, and the food industry. Over the past decade, immobilized enzymatic catalysis, as a green chemistry technique, has been employed to modify polysaccharide molecules and generate novel bioactive oligosaccharides. As instance, an immobilized enzyme reactor (IMER) system comprising two primary enzymatic compartments was constructed. The first compartment, consisting of a monolithic Convective Interaction Media® (CIM®) carboxy imidazole (CDI) disk with immobilized laccases (EC 1.10.3.2) from Trametes versicolor, was designed to introduce phenol groups into polysaccharides. Dextran T40, selected as a model polysaccharide, was used to evaluate the phenolization process. The second compartment was designed to break down polysaccharides, leading to the production of oligosaccharides. A CIM® CDI disk with immobilized glucuronan lyases (EC 4.2.2.14) from Rhizobium rosettiformans was employed to degrade glucuronan. In both compartments, the kinetic parameters of free and immobilized enzymes were quantified, including the maximum reaction rate (Vmax) and the Michaelis constant (Km). To optimize enzymatic catalysis, design of experiments (DOE) and response surface methodology (RSM) were applied to investigate the effects of key operating parameters, i.e., substrate concentration, flow rate, and reaction time. The stability of the immobilized enzyme reactor was also monitored to assess its lifespan. Finally, we aim to integrate these two compartments with a membrane filtration system to develop a multistep enzymatic reactor for the controlled processing of poly- and oligosaccharides.*

Key words: Immobilized enzyme reactor (IMER), polysaccharide modification, bioactive oligosaccharides, Design of experiments (DOE), Green biocatalysis

* Corresponding author: guillaume.pierre@uca.fr

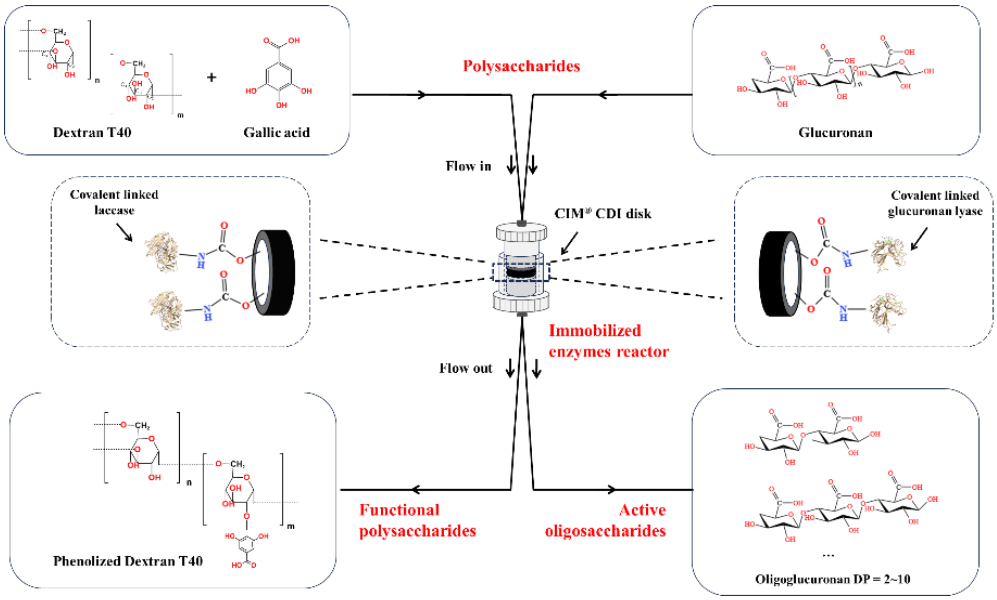


Figure 1. Schematic diagram of CIM® CDI monolithic reactors immobilized with laccases or glucuronan lyases for producing functional polysaccharides or active oligosaccharides, respectively.

Dr. Guillaume Pierre has been an Associate Professor at Université Clermont Auvergne since 2011 and, since 2023, a Junior Chair in Innovation at the Institut Universitaire de France (IUF), a distinction that recognizes researchers for excellence and innovation potential.

His research at the Institut Pascal (GePEB group, Team 4Bio) focuses on bioprocess engineering and the valorization of polysaccharides and bio-based functional molecules, bridging chemistry, biotechnology, and process sciences. He has authored more than 116 peer-reviewed publications, 11 book chapters, and 6 patents (h-index: 41), and has supervised 8 PhD students, 6 postdoctoral fellows, and 17 master's students.

His projects have secured over €1 million in national and international funding, including the ANR RAh project (2023–2028), the CMA-BIORAF program (2024–2029), and the PHC MAGHREB EXPLORE program (2019–2022). Dr Pierre currently serves as Head of the Biological Engineering Department at Polytech Clermont, is an elected member of the French National Council of Universities (CNU, Section 64) and sits on the editorial boards of several scientific journals. He is also an expert reviewer for national and international calls, received the French Glycosciences Society Young Researcher Award (2022), and is regularly invited as a keynote speaker or visiting lecturer in Japan, Sweden, Italy, and North Africa. His work lies at the crossroads of bioprocess innovation, sustainable bioresources, and industrial biotechnology, combining scientific excellence with educational leadership and international collaboration.

PL13 THE ROLE OF ARTIFICIAL INTELLIGENCE IN PHYTOTHERAPY

Anca Daniela Raiciu[1,2,3] *

[1]"TITU MAIORESCU"University, Faculty of Pharmacy, Pharmacognosy, Phythochemie, Phythoerapy, Gh. Sincai Street no. 16, district 4, Bucharest, 040315,Romania

[2]PLANTA ROMANICA Associaton,George Enescu street, no.27-29;district 1;Bucharest; 010303, Romania

[3]Hofigal Export-Import S.A.; Intrarea Serelor no. 2; district 4; Bucharest; 042124, Romania

Abstract:*Artificial Intelligence (AI) plays an increasingly significant role in phytotherapy by accelerating the identification of bioactive compounds, optimizing extraction and formulation processes, and improving quality control.Through advanced data analytics and predictive modeling, AI enables personalized phytotherapeutic approaches and evidence-based validation, bridging traditional botanical knowledge with modern computational methods to enhance therapeutic efficacy and safety.*

Key words: Artificial intelligence, phytotherapy, machine learning, medicinal plants, bioactive compounds, data analysis, personalized medicine

Introduction: Phytotherapy uses medicinal plants to prevent and treat various diseases. The integration of Artificial Intelligence (AI) offers new opportunities for improving this traditional field. AI can analyze complex biological data and identify active compounds more efficiently. It supports personalized treatments and enhances research accuracy. Combining AI with phytotherapy bridges tradition and innovation. This synergy promotes safer and more effective natural therapies.

Experimental and/or Modelling: The study applied AI-based data analysis to identify medicinal plants with potential therapeutic effects. Databases containing phytochemical structures and biological activities were processed using machine learning algorithms. Models were trained to predict bioactivity and optimize extraction parameters. The AI system evaluated correlations between compounds and targeted diseases. Experimental validation confirmed the predicted activities. The combined approach improved efficiency and accuracy in phytotherapeutic research.

Results and discussions: The AI-based analysis successfully identified several plant species with high predicted bioactivity against inflammation, diabetes, and microbial infections. Machine learning models demonstrated strong predictive accuracy when compared with experimental validation data. Figure 1 illustrates the correlation between predicted and observed biological responses, confirming the model's reliability. AI algorithms also optimized extraction parameters, resulting in higher yields of active compounds. Data clustering revealed chemical similarities

* Corresponding author: daniela_raiciu@yahoo.com

among different plant extracts, facilitating the classification of phytotherapeutic agents. Moreover, AI supported the identification of potential drug–plant interactions, improving treatment safety. The integration of computational predictions with laboratory validation enhanced research efficiency. Overall, the results demonstrate that AI can significantly accelerate discovery and development in phytotherapy**.**

Conclusions: Artificial Intelligence significantly enhances phytotherapy by accelerating the discovery of bioactive compounds and improving treatment personalization. Its integration ensures a more efficient, accurate, and evidence-based approach to natural medicine.

References:

1. Ahmad, M., & Rahman, M.,**2023**,*Artificial intelligence applications in herbal medicine research: Current trends and future perspectives,*Frontiers in Pharmacology, 14, 1123456
2. Dey, A., & Mukherjee, P. K.,**2022,***Role of computational tools and artificial intelligence in phytochemical research*,Phytomedicine, 99, 154024
3. Feng, X., Zhang, Y., & Li, C.,**2021**,*Machine learning approaches for predicting bioactive compounds from medicinal plants,*Journal of Ethnopharmacology, 275, 114098
4. Khatri, P., Kumar, N., & Singh, R.,**2020**,*Integration of artificial intelligence and natural product research: A systematic review*,Computers in Biology and Medicine, 127, 104058
5. Liu, J., Chen, W., & Wang, Y.,**2023**,*Deep learning-based screening of phytochemicals for therapeutic potential*.* **Computational and Structural Biotechnology Journal, 21, 4567–4579
6. Mukherjee, P. K., & Houghton, P. J.,**2021***,The future of herbal medicine: Artificial intelligence and big data integration,*Journal of Herbal Medicine, 27, 100424
7. Rajput, S., & Sharma, R.,**2022**,*Artificial intelligence in pharmacognosy and drug discovery from plants*, Artificial Intelligence in Medicine, 130, 102338
8. Zhao, L., Xu, M., & Chen, H.,**2024**,*AI-driven modeling for personalized phytotherapy: Advances and challenges,*Frontiers in Artificial Intelligence, 7, 145623

BOOK OF ABSTRACTS

SICHEM – 2025

A – Chemical and biochemical engineering (CBE)

1. Keynotes

SA-KN01 PHOTOCATALYTIC AND PHOTO-PHOTOELECTROCHEMICAL RECOVERY OF RESOURCES AND CRITICAL METALS: TOWARD A CIRCULAR ECONOMY

Ridha Djellabi*

Department of Chemistry, Alfaisal University, Al Zahrawi Street, Al Maather, Al Takhassusi Road, Riyadh, 11533, Saudi Arabia

Abstract: *In line with Zero Waste and circular economy principles, recovering resources and critical materials from wastewater is an effective strategy for preserving natural capital and preventing environmental harm. Most current strategies focus on conventional water treatment, emphasizing pollutant removal or oxidation rather than recovering them for reuse. Municipal and industrial wastewaters are rich with a lot of resources and critical metals that need to be extracted. In this talk, we will discuss the simultaneous purification of industrial wastewater along with resources recovery via photocatalytic and photo(electro)deposition mechanism. In photocatalysis, a simple photocatalyst is used which activated light irradiation, allowing excitation and the generation redox system. This latter leads to recovering metals in water such as Cr(VI), Ni(II) and Ag(I) exist in wastewater via deposition which then can be extracted from the surface for further reuse. In photoelectrochemical, the synergism of photocatalysis and electrochemical is obtained, resulting in powerful system to detoxify wastewater and recovery of resources such as metallic and nutrient species via deposition or/and by precipitation at lower power consumption compared to single electrochemical process. These practices help preserve natural capital, prevent the environmental impacts of these materials, and offer significant economic advantages over traditional purification systems.*

Key words: Solar photocatalysis, Photoelectrochemical process, Critical metal recovery, Resources recovery, Photodeposition, Zero Waste, Circular economy.

References:

[1] Djellabi, Ridha, et al. Carbonaceous biomass-titania composites with Ti-O-C bonding bridge for efficient photocatalytic reduction of Cr(VI) under narrow visible light. Chemical Engineering Journal, 2019, vol. 366, p. 172-180.

[2] Djellabi, Ridha, et al. Cr(VI) photocatalytic reduction under sunlight followed by Cr(III) extraction from TiO_2 surface. Materials Letters, 2016, vol. 176, p. 106-109.

[3] Djellabi, R., et al. Advances in photocatalytic reduction of Cr(VI): from fundamental concepts to materials design and technology challenges. J Water Process Eng 50: 10330, 2022.

[4] Qiao, M., Wu, X., Zhao, S., Djellabi, R., & Zhao, X. (2020). Peroxymonosulfate enhanced photocatalytic decomposition of silver-cyanide complexes using g-C_3N_4 nanosheets with simultaneous recovery of silver. Applied Catalysis B: Environmental, 265, 118587.

[5] Zhang, J., Zhao, X., Wang, Y., & Djellabi, R. (2019). Recovery of phosphorus from hypophosphite-laden wastewater: a single-compartment photoelectrocatalytic cell system integrating oxidation and precipitation. Environmental Science & Technology, 54(2), 1204-1213.

[6] Zhang, J., Djellabi, R., Zhao, S., Qiao, M., Jiang, F., Yan, M., & Zhao, X. (2020). Recovery of phosphorus and metallic nickel along with HCl production from electroless nickel plating effluents: The key role of three-compartment photoelectrocatalytic cell system. Journal of hazardous materials, 394, 122559.

* Corresponding author: rdjellabi@alfaisal.edu

BOOK OF ABSTRACTS

SICHEM – 2025

A – Chemical and biochemical engineering (CBE)

2. Oral presentations

SA-OP01 APPLICATION OF NEW CHELATING RESIN IN BRINE HARDNESS REMOVAL TO FEED THE CHLOR-ALKALI MEMBRANE CELL PROCESSVII. THERMODYNAMIC AND KINETIC STUDIES

Valeria Danilova, Dumitru Coman, Liliana Lazăr*, Ioan Mămăligă

"Gheorghe Asachi" Technical University of Iasi, "Cristofor Simionescu" Chemical Engineering and Environmental Protection Faculty, 73 Prof. Dimitrie Mangeron Street, 700050, Iasi, Romania

Abstract**:** *This paper presents the experimental results obtained in the laboratory for the thermodynamic and kinetic analysis of the brine purification process by ion exchange using a relatively new resin, specialized for the chlor-alkali industry.*
Key words: brine electrolysis, ion exchange resins, secondary brine purification ultrapure brine

Introduction: The use of zero-gap membranes for chlor-alkali industry requires the continuous optimization of the secondary brine purification process through ion exchange to ensure the technological and energy performance of industrial electrolyzes. Supplying electrolyzes with saturated and ultrapure brine ensures high current efficiency and minimal energy consumption [1,2]. Commercial polymeric resins in the sodium form are used industrially for the selective removal of alkaline earth cations in secondary brine purification by ion exchange for the production of high-purity brine in the chlor-alkali electrolysis process [2,3].

Experimental: For laboratory studies, a weakly acidic cation exchange resin with chelating iminodiacetic acid groups the commercial ion exchanger Lewatit® MonoPlus TP 208 resin by Lanxess is used. In the experiments both industrial brine with initial concentration of NaCl about 320g/L and synthetic solutions (calcium chloride and magnesium chloride solution) with concentration in calcium of approx. 0,6 mg/L were used. The removal of Ca^{2+} and Mg^{2+} ions experiments were investigated in batch operation type. The experiments were performed by introducing a precisely weighed amount of ion-exchange resin into a volume of 50 mL of liquid phase at the different condition to work, then the mixture was filtered and analysed to determine the total hardness, Ca^{2+} and Mg^{2+} concentration, NaCl concertation and optimal ion exchange resin dose for hardness removal. ATR-FTIR spectra were recorded using a Bruker Vertex 70 FTIR spectrometer (Bruker Optics, Ettlingen, Germany) for the direct analysis of solid sample surfaces for comparative studies on the ion exchange resin, the initial commercial form and the used form, after exhaustion of the regeneration cycles.

Results and discussions: The industrial exploitation of ion exchange resin based on the data in the product data sheet does not always lead to the desired results, and

* Corresponding author: liliana.lazar@academic.tuiasi.ro, lillazar@ch.tuiasi.ro

resin depletion can be prevented by establishing a technological regime depending on the rock salt and the concentration of brine used in the industrial process. The ATR-FTIR analysis demonstrated notable changes in the intensity and position of characteristic absorption bands corresponding to functional groups such as C=O and N–H, reflecting chemical degradation of the active sites within the resin matrix. These spectral modifications are attributed to complex interactions between the resin and different ions, as well as water adsorption during the ion exchange and regeneration cycles. Collectively, these changes contribute to a significant decrease in the ion exchange capacity of the used resin compared with the initial, unused material, highlighting the impact of operational conditions on resin performance and longevity. For the main phase of experiments, the effect of different operational factors including, ion-exchange resin dose, temperature, initial brine hardness, contact time solid – liquid on the practical ion exchange ability was also investigated.

Conclusions: This study is justified by the need to adopt and optimize the industrial process for purifying brine used for electrolysis in ion exchange membrane cells. The kinetics followed the pseudo-second-order kinetic model ($R^2 > 0.985$) for brine and synthetic solutions. Equilibrium data were fitted to Langmuir and Freundlich isotherm models with Langmuir model providing a slightly better predication ($R^2 > 0.985$). The model prediction was in good agreement with observed data ($R^2 = 0.99$). This preliminary study allows for the next subsequent implementation of the ion-exchange brine purification process in dynamic mode.

Acknowledgement: This work was supported by a National Research Grant (ARUT), Project number GNaC 2023-274/2024 and the Doctoral School of the "Gheorghe Asachi" Technical University of Iasi, Romania.

References:

[1] Thyssenkrupp, Uhde Chlorine Engineers, *Industrial Solutions Chlor-Alkali Electrolysis Three Best-in-Class Technologies* (http://www.thyssenkrupp-uhde-chlorine-engineers.com/; accessed September 2025).

[2] O'Brien T.F., Bommaraju T.V., Hine F., *Handbook of Chlor-Alkali Technology*, Springer. 2004.

[3] Bayrama Y., Removal of major impurties (Ca-Mg) of brine with chemical treatment process in the salt sector, *International Scientific and Vocational Journal,* 2, (2018),57-66.

SA-OP02 PRELIMINARY STUDY REGARDING THE ETHANOL PRODUCTION FROM A MIXTURE OF BANANA, ORANGE AND MELON PEEL

Estera Vasilescu[1], Alexandru-Cristian Vîlcică[1], Edna Adriana Anton[1], Gabriel-Marius Cioroiu[2], Liviu-Constantin Stan[2] and Doinița-Roxana Tîrpan*

[1] Ovidius University of Constanta, Chemistry and Chemical Engineering Department, 124 Mamaia Blvd., 900527, Constanta, Romania

[2] Faculty of Naval Electromechanics, Department Electromechanics, Constanta Maritime University, 104 Mircea cel Batran Blvd, 900663, Constanta, Romania

Abstract: *In this study was performed the production of second generation bioethanol from fruit waste.* ***Key words:*** Bioethanol, biomass, fermentation

Introduction: Bioethanol represents the biofuel extracted from biomass or from the biodegradable part of vegetable wastes. This renewable biofuel has a small calorific power, an octane number 111 and freezing point -114 °C. It can completely replace gasoline, more successfully than biomethanol, a solution adopted in some countries with high sugarcane production like Brazil but the carbureted engine must be modified.

Experimental: Our work is focused on the production of second generation bioethanol from fruit waste, namely orange (*Citrus sinensis*), banana (*Musa acuminate*) and melon (*Cucumis melo var. cantalupensis*) peel. The choice of this mixture is based on a relatively accessible biomass, it does not compete with other industries and it has reasonable amounts of sugars to be treated: orange peel (2,3% glucose, 3,5% sucrose, 2,7% fructose), banana peel (4% glucose, 6% sucrose, 2,7% fructose), melon waste (1% glucose, 5% sucrose, 2% fructose).

Results and discussions: In our process protocol, the physical treatment was divided in 3 steps: cutting the fruit peels into smaller pieces, thermically treating them in the oven, grinding them into smaller pieces with an electrical chopper. The thermal treatment occurred at a temperature of 150ºC for 180 minutes, time in which the biomass was observed and checked several times, in order to prevent over-cooking, event that could have damaged the sugar contents of the peels, therefore interfere with the yield of our next processes. The chemical preparation fraction is divided into hydrolysis and alcoholic fermentation. More exactly, a low-concentration acid hydrolysis (H_2SO_4, 1%) was followed by an anaerobic fermentation with *Saccharomyces cerevisiae.* Then, the fermented hydrolysate was introduce in a distillation apparatus.

Conclusions: The yield of bioethanol obtained was 30 % proving that is a viable alternative method in biofuel production.

References:

[1] Setiawan H. *et al.*, *Optimized supply chain of empty fruit bunches as feedstocks for second generation bioethanol production,* Case Studies in Chemical and Environmental Engineering, Volume 10, December 2024, 100950.

* Corresponding author: tirpanroxana@gmail.com

SA-OP03 FROM SIMULATION TO SAFETY: CHEMICAL RISK MANAGEMENT AND ENVIRONMENTAL SAFETY IN EUROPEAN CIVIL PROTECTION EXERCISES

Alexandra-Ioana Crăciun[1,2,*], Alexandru Ozunu[1,2]

[1]Babeş-Bolyai University of Cluj-Napoca, Faculty of Environmental Science and Engineering (FSIM), Doctoral School of Environmental Science, 30 Fântânele Street, RO-400294, Cluj-Napoca, Romania

[2] Research Institute for Sustainability and Disaster Management based on High Performance Computing (ISUMADECIP), Babeș-Bolyai University, 30 Fântânele Street, RO-400294, Cluj-Napoca, Romania

Abstract*: The increasing complexity of chemical, biological, radiological, and nuclear (CBRN) emergencies within Europe requires continuous enhancement of preparedness, coordination, and interoperability across national and international response structures. Within the framework of the Union Civil Protection Mechanism (UCPM), the EU MODEX field exercises serve as key operational platforms for improving cooperation, coordination, and decision-making during complex, multinational deployments.*

This paper presents a comparative operational analysis of two CBRN-oriented exercises: EU MODEX Lyon 2023 (France) and EU MODEX Riga 2025 (Latvia), both focused on chemical detection and sampling missions conducted under simulated emergency conditions. The study highlights how realistic CBRN scenarios, structured injects, and international collaboration enhance the preparedness of participating modules to operate in a foreign environment, in accordance with UCPM standards and procedures. The Lyon 2023 exercise simulated an industrial accident caused by a severe storm affecting multiple SEVESO-classified facilities along the Rhône corridor, requiring international assistance for chemical risk assessment and coordination. The Riga 2025 exercise, conducted during the EuroBasket international sports event, was based on the pre-positioning of specialized CBRN teams to support host nation authorities through detection, sampling, and analysis of hazardous substances in crowded urban settings.

Both exercises integrated realistic simulation techniques, including scripted events, injects, and dynamic scenario development, that allowed participants to train decision-making, communication, and operational coordination. The Environmental Impact Assessment (EIA) process conducted in Riga provided an additional operational layer, ensuring that all simulated activities were aligned with safety standards, environmental protection measures, and host nation legislation.

From an operational perspective, both exercises demonstrated the importance of harmonized procedures for CBRN detection and sampling, effective safety management (including "NO PLAY" protocols), and compliance with environmental and health standards. The results underline that structured simulations, rather than purely technical trials, are essential for validating coordination, field logistics, and communication mechanisms within international CBRN interventions.

The findings confirm that EU MODEX CBRN exercises function as applied simulation environments that strengthen interoperability, improve preparedness, and enhance environmentally responsible field operations. By bridging simulation-based training and operational response, these exercises contribute to building a more resilient European Civil Protection framework capable of addressing complex chemical and radiological risks.

Key words: CBRN, chemical risk management, detection and sampling, environmental safety, civil protection, EU MODEX, interoperability, UCPM, operational preparedness.

*Corresponding author: alexandra.craciun@ubbcluj.ro

SA-OP04 SYNTHESIS OF HIGHER ALCOHOLS WITH POTENTIAL APPLICATIONS IN COSMETICS INDUSTRY: PROCESS ANALYSIS

Andreea Manolache, Ionut Banu, Ana-Maria Brezoiu, Oana Pârvulescu, Adina Gavrilă

Faculty of Chemical Engineering and Biotechnologies, POLITEHNICA Bucharest, 1-7 Gh. Polizu, 011061, Bucharest, Romania

Abstract: *Alcohols are widely used as solvents in the cosmetics industry due to their ability to dissolve active ingredients and enhance product stability. Ethanol is the common choice for formulations used in perfumes, toners or hand sanitizers, offering quick-drying effects and antimicrobial properties. In this work, a conceptual design of an alcohols synthesis process with potential applications in cosmetic industry was carried out, especially for ethanol production.*
Key words: Syngas, ethanol, solvent, cosmetic formulation, economic evaluation, schedule

Introduction: Ethanol is a primary alcohol that has multiple uses in practice: acts as an antiseptic, a polar solvent, a neurotoxin, a central nervous system depressant and a disinfectant. Moreover, it is widely employed in cosmetic formulations as a solvent, antimicrobial agent, and penetration enhancer, contributing both to product stability and efficiency [1].

Modelling: In the proposed process, higher alcohols are being produced through syngas chemical conversion in a continuous reactor, in the presence of an alkali-Co doped MoS_2 catalyst [1]. A process flowsheet was proposed, heat and mass balances evaluated, and equipment preliminary sizing performed using Aspen Plus v14. Further, a time schedule and cost estimate for a conceptual phase project which concluded with a business case evaluation was investigated. The project scenario was subjected to a comprehensive assessment including an economic evaluation based on rigorous business case calculations, a Class 5 cost estimate to reflect early-stage accuracy levels, and the development of a detailed project timeline in Microsoft Project.

Results and discussions: The process flowsheet could be divided into five sections: reaction, gas-liquid separation, water removal, alcohol separation and purification. Methanol, ethanol and n-propanol were obtained as main products. The project capital expenditure (CAPEX) was estimated according to Happel's methodology for Class 5 cost estimates [2], considering a total project duration of 5 years and 9 months.

Conclusions: An economic feasibility of the proposed process was assessed, and the following indicators were calculated: internal rate of return (IRR)=15.88 % and discounted payback period (DPP) = 10.5 years.

References:

[1] Portillo, M.A., Perales, A.L.V., Vidal-Barrero, F., Campoy, M., „A kinetic model for the synthesis of ethanol from syngas and methanol over an alkali-Co doped molybdenum sulfide catalyst: Model building and validation at bench scale", Fuel Processing Technology, 151, 2016, pp.19-30

[2] Happel, J., Jordan, D. G., "Chemical process economics", M. Dekker, New York, Second edition, 1975.

SA-OP05 ON THE SEPARATION OF VEGETABLE OILS INTO COMPONENT CLASSES

Nicoleta-Oana Demostene[1,*], Petrica Iancu[1], Roxana Tarpan[2], Tănase Dobre[1]

[1]National University of Science and Technology POLITEHNICA Bucharest, 1-7 Gheorghe Polizu Str., 011061 Bucharest, ROMANIA

[2]Universitatea Ovidius Constanta, 124 Mamaia Boulevard, 900527 Constanța, ROMANIA

Abstract: *This study investigates the separation of vegetable oils into distinct classes of components using both conventional and modern techniques. Starting from crude vegetable oil, numerous value-added compounds can be recovered, many of which are associated with health-promoting properties such as antioxidant and anti-inflammatory effects. The paper presents traditional refining and fractionation methods, alongside emerging technologies such as membrane separation and supercritical fluid extraction (SC-CO_2). Each technique is analyzed in terms of its efficiency, environmental impact, and economic feasibility. Comparative evaluation highlights that modern methods offer higher selectivity and lower energy consumption, while traditional processes remain advantageous for large-scale applications due to their lower operational costs. Overall, this work provides an integrated perspective on the technological potential of separating vegetable oils into functional fractions for use in the food, pharmaceutical, and cosmetic industries.*

Key words: vegetable oils, oil fractionation, chemical refining, physical refining, modern separation techniques, bioactive compounds

Introduction: Vegetable oils play a crucial role not only in daily nutrition but also as key raw materials across various industries, including food, leather, paint, rubber, textiles, cosmetics, and pharmaceuticals. For the valorization of vegetable oils, it is possible to resort to their fractionation and separation into distinct classes of compounds, having specific properties and applications. Refining vegetable oils removes impurities while preserving bioactive compounds [1]–[3].

Chemical Composition of Vegetable Oils: The composition of triacylglycerols, monoacylglycerols, and diacylglycerols varies depending on the type of vegetable oil. Fatty acids are the fundamental constituents of triglycerides. The composition of vegetable oils includes both beneficial substances and undesirable components, the latter of which must be removed to obtain a high-quality, stable oil. Desirable constituents include triacylglycerols, tocopherols, squalene, and phytosterols. Conversely, phospholipids, free fatty acids, hydroperoxides, heavy metals, and moisture are considered undesirable, negatively affecting oil stability and quality [1], [4].

Vegetable Oil Separation Methods: During refining, the classes of constituents that impair oil quality are removed, but other compounds with potential health benefits, which could be further valued, are also eliminated. The traditional refining methods are chemical and physical. Chemical refining is carried out in six stages:

* Corresponding author: Email address:

degumming, neutralization, washing and drying, bleaching, dewaxing, and deodorization, whereas physical refining encompasses all the stages of chemical refining except for the neutralization step [5]. There are also advanced separation methods, such as membrane technology, dry fractionation (winterization), and supercritical fluid extraction [6]–[8].

Health benefits of vegetable oils: Vegetable oils exhibit anti-inflammatory properties, helping to counteract diseases associated with chronic inflammation, reduce the risk of cardiovascular disorders, demonstrate anticancer effects, and offer additional health benefits [1], [9].

Industrial Applications: Vegetable oils and their fractions have numerous applications at the industrial level. Vegetable oils and their fractions are extensively used as frying media in both domestic cooking and food manufacturing, including products such as snack chips, cookies, pastries, doughnuts, and fried potatoes, in the production of margarine and pastry products [10], [11].

Conclusions: Traditional and modern methods separate vegetable oils into valuable fractions, with advanced techniques offering more sustainable and selective recovery of bioactive compounds.

References:

[1] M. Tian, Y. Bai, H. Tian, and X. Zhao, The Chemical Composition and Health-Promoting Benefits of Vegetable Oils- A Review, *Molecules*, 28, 17, (2023).

[2] S. C. Chew and K. L. Nyam, Refining of edible oils, *Lipids and Edible Oils: Properties, Processing and Applications*, Elsevier Inc., (2020), 213–241.

[3] N. J. Oswell, F. D. Gunstone, and R. B. Pegg, "Vegetable oils," in *Bailey's Industrial Oil and Fat Products*, 2020.

[4] N. J. Oswell, F. D. Gunstone, and R. B. Pegg, Vegetable oils, *Bailey's Industrial Oil and Fat Products*, (2020).

[5] A. Sonawane and S. Waghmode, A Review on Vegetable Oil Refining: Process, Advances and Value Addition to Refining by-Products, *Bioremediation for Global Environmental Conservation*, (2023).

[6] C. de Morais Coutinho, M. C. Chiu, R. C. Basso, A. P. B. Ribeiro, L. A. G. Gonçalves, and L. A. Viotto, State of art of the application of membrane technology to vegetable oils: A review, *Food Res. Int.*, 42, 5–6, (2009), 536–550.

[7] O. Zaliha, C. L. Chong, C. S. Cheow, A. R. Norizzah, and M. J. Kellens, Crystallization properties of palm oil by dry fractionation, *Food Chem.*, 86, 2, (2004), 245–250.

[8] O. Dhara, K. N. P. Rani, and P. P. Chakrabarti, Supercritical Carbon Dioxide Extraction of Vegetable Oils: Retrospective and Prospects, *Eur. J. Lipid Sci. Technol.*, 124, 8, (2022).

[9] N. Shahzad *et al.*, Phytosterols as a natural anticancer agent: Current status and future perspective, *Biomed. Pharmacother.*, 88, (2017), 786–794.

[10] S. W. Lin, Palm Oil, *Vegetable Oils in Food Technology: Composition, Properties and Uses*, (2011), 25–58.

[11] D. B. Yayla, Vegetable Oil Fractionation : Technological Methods , Applications , and Future Perspectives, *ZEUGMA Biol. Sci.*, 6, 1, (2025), 1–13.

SA-OP06 DECENTRALIZED MODEL PREDICTIVE CONTROL OF THE NITRIFICATION AND DENITRIFICATION PROCESSES IN THE WASTEWATER TREATMENT PLANT

Adrian G. Bodescu[1,*], Romina G. Dărăban[1], Vasile M. Cristea[1]

[1]Babeş-Bolyai University, Department of Chemical Engineering, Cluj-Napoca

Abstract: *Model predictive control (MPC) represents a set of advanced control methods that utilize a process model to forecast the future behavior of the controlled system. This control method has been implemented in wastewater treatment plants for control of the dissolved oxygen (DO) in the aerated reactor, by manipulating the air flow, coupled with control of the nitrate and nitrite nitrogen (NO) concentration in the anoxic reactor, by manipulating the internal recycle. The MPC controllers achieved good control performance with zero offset, small overshoot and by promptly counteracting the strong influent disturbances.*

Key words: Model Predictive Control, Wastewater treatment plants, Activated sludge model no. 1.

Introduction: The pollution prevention of natural resources by wastewater, along with the adequate implementation of wastewater treatment (WWT) before reuse, are crucial factors in developing and designing effective wastewater disposal systems [1]. These systems can be investigated using models able to describe the performance of WWTP carrying out carbon oxidation, nitrification, and denitrification, namely the Activated Sludge Model No.1, further use in model based control. [2]

Modelling and Control Methodology: The Benchmark Simulation no 1. has been used as the starting point for modeling and calibration of the Anaerobic-Anoxic-Oxic municipal WWTP, and Matlab/Simulink as the simulation software. As inputs, data from the municipal wastewater treatment plant of Cluj Napoca, Romania was utilized. Multiple step dynamic simulation scenarios have been created for transfer function model identification, further used in MPC design. The two single input-single output models, having as inputs the air flow rate and NO recycle flowrate, and as outputs the DO and NO concentration were considered. These models served as the basis for the MPC controller design and tuning.

Results and discussions: For testing, different setpoint SP values have been given to the MPC controllers and their performance was observed for both setpoint tacking and disturbance rejection. The following figures illustrate the control results for each of the 2 MPC structures investigated. They show the ability of the MPC to counteract the WWTP influent disturbances.

* Corresponding author: adrian.bodescu@ubbcluj.ro

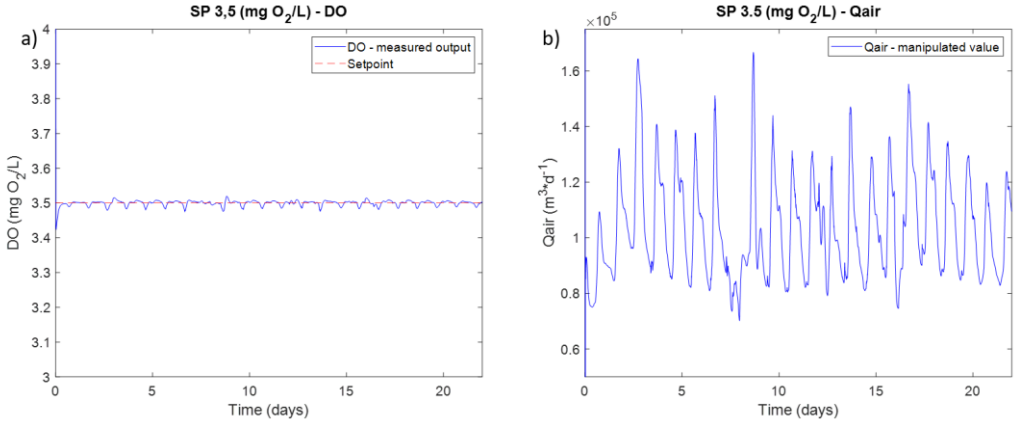


Fig. 1. MPC controlled output (a) and manipulated value (b) for DO control at SP = 3.5 [mg O_2/L]

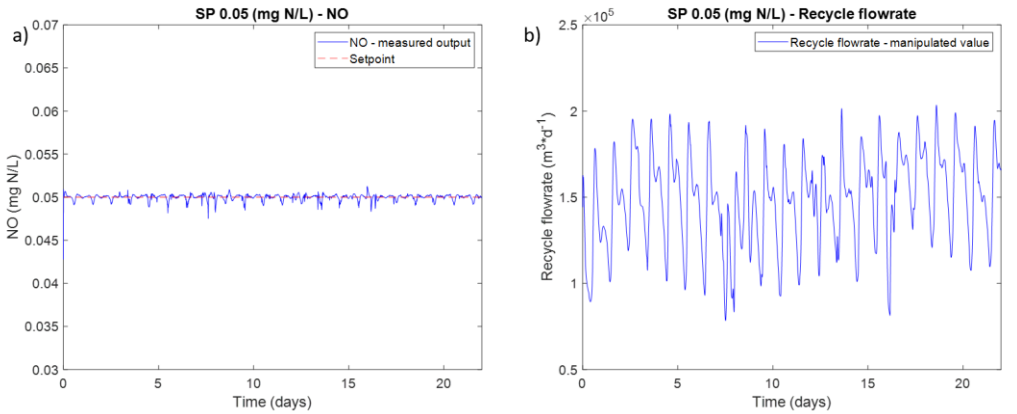


Fig. 2. MPC controlled output (a) and manipulated value (b) for NO concentration control at SP = 0.05 [mg N/L]

Conclusions: Both designed MPC controllers succeeded to achieve good control performance, with zero offset, small overshoot and promptly counteracting the strong influent disturbances. They demonstrate good potential for municipal plant application.

References:

[1] Kumar K., Pitta S., Babu J., Performance evaluation of wastewater treatment plant, Int. J. Eng. Sci. Tech, 2, (2010),7785-7796.

[2] Jeppsson U., A General Description of the IAWQ Activated Sludge Model No. 1. Modelling aspects of wastewater treatment processes, PhD thesis, Lund University, Lund, Sweden, 1996.

SA-OP07 MONITORING OF THE DIESEL HYDRODESULFURIZATION REACTOR AND PRIMARY STATISTICAL DATA EXPLOITATION

Laura Elisabeta Petras[1,2*], Claudia Muntean[3], Tănase Dobre[1]

[1]Chemical and Biochemical Engineering Department, University POLITEHNICA Bucharest, 1-7 Gheorghe Polizu Str., 011061 Bucharest

[2]Petromidia Refinery, NavodariBld 214, Navodari 905700

[3]Chemistry and Chemical Engineering Department, Ovidius University 124 Mamaia Bld 900527

Abstract: *This paper presents the monitoring and statistical evaluation of an industrial diesel hydrodesulfurization (HDS) reactor operated under steady-state conditions. Process variables such as temperature, pressure, hydrogen circulation, and product sulfur concentration were continuously recorded by the refinery's Distributed Control System (DCS). The collected data were processed using statistical tools to determine correlations between key parameters and product quality. Strong dependencies were found between reactor temperature, hydrogen-to-oil ratio, and outlet sulfur concentration. Simulation studies confirmed the statistical trends and validated process sensitivity to operational changes. The combined monitoring and simulation approach provides a reliable basis for predictive control and process optimization in diesel hydrotreating units.*

Key words: Diesel hydrodesulfurization, process monitoring, statistical analysis, refinery optimization, sulfur removal.

Introduction: Diesel hydrodesulfurization (HDS) is an essential catalytic process used to remove sulfur compounds from middle distillates to meet ultra-low sulfur specifications. Maintaining process efficiency and catalyst performance requires continuous monitoring and data-driven optimization. The present study focuses on industrial monitoring of an HDS reactor, highlighting correlations among key parameters and their influence on product sulfur levels [1-5].

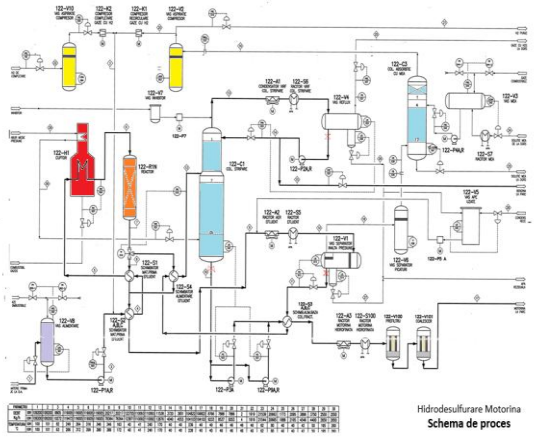


Figure 1. *Schematic representation of the industrial diesel HDS reactor and monitoring system*

* Corresponding author: laurapetras@yahoo.com

Experimental and/or Modelling: The study was conducted on an industrial HDS reactor processing a blend of straight-run diesel and light cycle oil. The Distributed Control System (DCS) continuously recorded inlet/outlet temperatures, reactor pressure, liquid feed flow, hydrogen circulation rate, and product sulfur concentration. The collected data were statistically processed using Excel and MATLAB. Regression models were developed to describe the relationship between operational parameters and desulfurization efficiency. Complementary simulations were carried out in ASPEN Plus using a pseudo-first-order kinetic model to validate the experimental trends [5-10].

Results and discussions: Statistical analysis revealed strong negative correlations between temperature and product sulfur concentration ($r \approx -0.82$) and between hydrogen-to-oil ratio and sulfur content ($r \approx -0.65$), confirming their dominant influence on conversion efficiency. Increasing reactor temperature from 315 °C to 335 °C resulted in approximately 25% lower sulfur content. Higher space velocity (LHSV) decreased desulfurization performance by about 15%. Simulated results agreed with monitored data, showing deviations below 5%. The integrated monitoring–simulation methodology demonstrated high predictive accuracy ($R^2 > 0.9$) and provided a reliable diagnostic tool for process optimization.

Conclusions: Continuous monitoring and statistical processing of refinery HDS reactor data enable accurate evaluation of process stability and efficiency. The correlations identified between temperature, hydrogen flow, and sulfur removal provide a solid basis for predictive control. Simulation validated the observed trends, confirming the potential of data-driven optimization for improved catalyst performance and hydrogen management.

References:

[1] Jimenez F., Nunez M., Kafarov V. (2005). *Study and modeling of simultaneous hydrodesulfurization, hydrodenitrogenation and hydrodearomatization on vacuum oil hydrotreatment.* In: European Symposium on Computer-Aided Processes, Elsevier Science.

[2] Babich I. V., Moulijn J. A. (2003). *Science and technology of novel processes for deep desulfurization of oil refinery streams: A review.* Fuel, 82, 607–631.

[3] Chowdhury R., Pedernera E., Reimert R. (2004). *Trickle-bed reactor model for desulfurization and dearomatization of diesel.* AIChE J., 48, 126–135.

[4] Saajanlehto M., Uusi-Kyyny P., Alopaeus V. (2014). *Hydrogen solubility in heavy oil systems: experiments and modeling.* Fuel, 137, 393–404.

[5] Baloochy B., Shokri S., Marvasar A. M. (2010). *Design and implementation of simulator for hydrotreating reactor in RTO development.* Int. J. Chemical Engineering and Applications, 1(4), 287–293.

[6] Novaes L. R., Resende N. S., Salim V. M., Secchi A. R. (2017). *Modeling, simulation and kinetic parameter estimation for diesel hydrotreating.* Fuel, 209, 184–193.

[7] Wang S., Liu Q., & Zhang Y. (2019). *AI-based predictive control for hydroprocessing units.* Chemical Engineering Research and Design, 148, 22–35.

[8] Mederos F. S., Ancheyta J. (2007). *Mathematical modeling and simulation of hydrotreating reactors: cocurrent versus countercurrent operations.* Applied Catalysis A: General, 332, 8–21.

[9] Murali C., Voolapalli R. K., Ravichander N., Gokak D. T., Choudary N. V. (2007). *Trickle-bed reactor model to simulate the performance of a commercial diesel hydrotreating unit.* Fuel, 86, 1176–1184.

[10] Dobre T., Petras L. E. (2024). Industrial data-driven modeling of diesel HDS reactor performance. Romanian Chemical Engineering Society Bulletin, 75(2), 115–129.

SA-OP08 SIMULATION AND CALIBRATION OF THE MATHEMATICAL MODEL ASM2dISS FOR THE MUNICIPAL WASTEWATER TREATMENT PLANT OF CLUJ-NAPOCA USING WEST+

Romina G. Dărăban[1,*], Adrian G. Bodescu[1], Vasile M. Cristea[1]

[1]Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Cluj-Napoca, Romania

Abstract: *This study aimed to both build the simulator based on the mathematical model ASM2dISS for the municipal wastewater treatment plant Cluj-Napoca and to calibrate it using the data collected from the municipal wastewater treatment facility. The simulation tool was WEST+, which has been specifically tailored in order to perform dynamic modeling of wastewater treatment processes. Furthermore, plant design characteristics were considered and several operating parameters were selected, while the latter were dynamically calibrated using real data from the Cluj-Napoca wastewater treatment plant (WWTP). The dynamic calibration is based on three objective functions defined to minimize the mean square difference between the model and the facility's soluble COD concentration (CODs), total nitrogen concentration (TN) and nitrite and nitrate concentration (NO) in the effluent. Calibration results are in good agreement with the available WWTP measurements, opening further real plant optimization and control investigations.*
Key words: WWTP, ASM2dISS, WEST+, calibration.

Introduction: WWTPs play an important role in managing water quality effluents of municipalities, both from an environmental and from an economic and social point of view [1]. Therefore, due to the fact that treatment plants are large and complex systems and they are prone to very large and continuous disturbances, various studies have been carried out in order to better understand the processes that occur in a WWTP and propose solutions for improved performance. They imply the use of mathematical models and the development of reliable dynamic simulators.

Model calibration using experimental data: The data used in calibration were obtained from the Cluj-Napoca WWTP measurements acquired during May, 2016. Data was collected online and correlated to daily laboratory analysis, taking into account both the main WWTP influent and effluent streams characteristics. The software used in the simulation is WEST+, a specially developed tool for the simulation of WWTPs. The parameters calibration was performed in dynamic state and was based on three objective functions, namely, minimization of the squared difference between the actual plant measured data and the simulated data for the CODs, TN and NO effluent concentrations.

Results and discussions: Following calibration in WEST+, the dynamic simulation results were compared with the plant collected data of the effluent. The results show that the dynamic changes described by the calibrated simulator for the effluent concentrations follow appropriately the effluent changes measured from the real plant.

* Corresponding author: romina.daraban@ubbcluj.ro

The mean absolute percentage error (MAPE) for the simulations performed in WEST+ were computed. The for CODs, NO and TN concentrations in the effluent are presented in Table 1, together with the 14-day mean values of the concentrations measured at the WWTP of Cluj-Napoca.

Table 1. 14-days mean values for WEST+ and WWTP concentrations and MAPE

Day	CODs		NO		TN	
	WEST+	WWTP	WEST+	WWTP	WEST+	WWTP
1	3.90	3.95	4.20	3.76	5.34	5.69
2	4.67	4.63	4.92	5.65	6.12	8.66
3	4.89	5.36	4.62	4.95	5.84	7.58
4	4.88	5.15	4.72	4.60	5.93	7.02
5	4.81	5.05	4.62	4.58	5.83	6.99
6	4.71	5.00	4.50	4.57	5.69	6.98
7	4.05	4.78	3.43	2.93	4.53	4.41
8	4.03	4.66	3.80	3.75	5.01	5.69
9	4.48	4.84	4.06	3.98	5.27	6.04
10	4.78	5.00	4.09	4.01	5.31	6.08
11	4.81	4.91	4.23	3.56	5.47	5.38
12	4.67	5.25	4.16	3.13	5.31	4.71
13	4.53	5.12	3.81	2.79	4.99	4.17
14	4.52	4.98	3.97	2.68	5.17	3.99
Mean	**4.55**	**4.91**	**4.22**	**3.92**	**5.41**	**5.96**
MAPE	**7.33%**		**7.65%**		**9.22%**	

The calibration results are in agreement with the literature reported data, where MAPE ranges for are 10% - 25% for COD, 15% - 30% for TN and 15% - 25% for NO [2-3].

Conclusion: Within this study, the mathematical model ASM2dISS was calibrated for the WWTP of Cluj-Napoca using the simulation software WEST+. The calibration results are good and further studies are opened with the developed simulator. The future prospects of the study are to calibrate the model using new data that includes total phosphorus concentration, to evaluate the effluent quality, pumping energy, aeration energy and greenhouse gas emissions.

References:

[1] Simon-Várhelyi M., Cristea V.M., Brehar M. Efficient calibration methodology of the wastewater treatment plant model based on ASM3 and application to municipal wastewater. *Desalination and water treatment*, 189, (2020), 108–118.; **[2]** Peng L., Jiangbei Q., Yiliang H., Zhang B., Mengke P. Global calibration model of UV-Vis spectroscopy for COD estimation in the effluent of rural sewage treatment facilities. *RSC Advances*, 10, (2020), 20691-20700.; **[3]** Vukmirović, A., Obrovski, B., Vukmirović, S. Statistical tools for municipal wastewater treatment plant efficiency evaluation. *Int. J. Environ. Sci. Technol.* 22, (2025), 7095–7102.

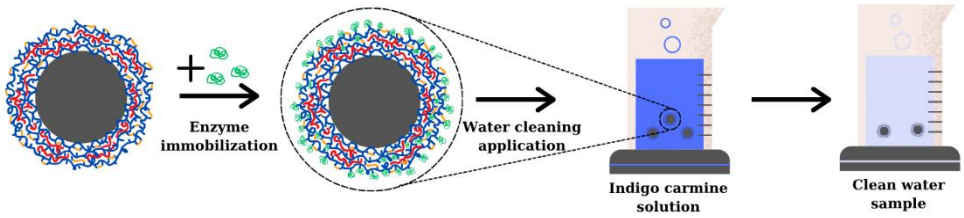
SA-OP09 ECO-FRIENDLY LACCASE/POLYELECTROLYTE/SILICA COMPOSITES WITH ENHANCED CATALYTIC ACTIVITY IN THE DEGRADATION OF WATER CONTAMINANTS

Larisa-Maria Petrila[1,*], Florin Bucatariu[1], Mihaela Silion[1], Rénato Froidevaux[2], Marcela Mihai[1]

[1]"Petru Poni" Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487, Iasi, Romania
[2] UMRt INRAE 1158 BioEcoAgro, Université de Lille, Avenue Paul Langevin 59655, Villeneuve d'Ascq, France

Abstract: *This study investigates a sustainable wastewater treatment approach utilizing immobilized enzymes for pollutant degradation. The employed method relies on the immobilisation of laccase on polyelectrolyte-based composite microparticles to obtain novel biocatalysts. The obtained biocatalysts were successfully utilized in the degradation of Indigo Carmine, serving as a model pollutant.*
Keywords: degradation, water treatment, laccase, Indigo Carmine, polyelectrolyte

Introduction: The increasing pollution of water, one of the most pressing challenges of recent years, has intensified the search for efficient technologies to degrade pollutants. Among the emerging technologies proposed, the use of immobilized enzymes has attracted considerable attention due to their natural origin, high catalytic specificity, and capacity to transform hazardous pollutants into less toxic compounds [1].
Experimental: *Reagents: Trametes versicolor* laccase, poly(ethyleneimine) (PEI) and poly(sodium methacrylate) (PMANa) were acquired from Sigma-Aldrich, and used as received. Silica microparticles were acquired from Daiso Co., and Indigo Carmine from VWR Chemicals. *Biocatalyst preparation:* The support microparticles for laccase immobilization were prepared by layer-by-layer deposition of PEI/PMANa on Daisogel microparticles. The immobilization of laccase was optimized following the effect of various parameters on the immobilization yield and catalytic activity. *Dye degradation studies:* The so-obtained biocatalysts were tested in the enzymatic degradation of Indigo Carmine in various conditions, assessing the effects of biocatalyst amount, dye concentration and pH on the catalytic process. Scheme 1 presents the experimental design, following (i) immobilization of laccase on the polyelectrolyte-coated silica microparticles and (ii) enzyme-catalyzed degradation of Indigo Carmine.



Scheme 1: Experimental set-up consisting of laccase immobilization on polyelectrolyte-based core-shell composite materials, followed by the catalytic degradation of Indigo Carmine in the presence of immobilized laccase

Results and discussions: In the initial set of experiments, the optimal conditions for laccase immobilization were determined. Both the initial enzyme concentration and the pH proved to be critical parameters for preserving enzymatic activity after immobilization. The obtained composites with immobilized laccase were subsequently employed as catalysts for the degradation of Indigo Carmine in various conditions. The obtained results demonstrated an increased efficiency of the biocatalysts in the dye degradation, achieving complete degradation under different dye concentrations and pH values [2]. Specifically, the biocatalysts were able to degrade Indigo Carmine at concentrations of 50 - 150 mg/L, with the highest degradation rate achieved at pH = 5.5, in line with the optimal pH for the immobilized laccase. Moreover, HPLC-MS was employed to identify the degradation products, evidencing the presence of less-toxic organic metabolites after enzymatic degradation.

Conclusions: The study proposes a sustainable and viable alternative to classical water treatment technologies, with emphasis on the use of enzymes as catalysts for the degradation of organic pollutants.

Acknowledgements: This work was financially supported by the Romanian National Authority for Research, with project number PNRR-III-C9-2022-I8-201, within the National Recovery and Resilience and by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-IV-P1-PCE-2023-1545, within PNCDI IV.

References:

[1] Chapman J., Ismail A. E., Dinu C. Z., Industrial applications of enzymes: Recent advances, techniques, and outlooks, *Catalysts,* 8 (2018) 238.

[2] Petrila L. M., Bucatariu F., Stoica I., Mihai M., Froidevaux R., A green approach combining polyelectrolyte-based core-shell microparticles and laccase for indigo carmine degradation. *J Environ Chem Eng,* 13 (2025) 115631.

SA-OP10 ASSESSMENT OF WWTP PERFORMANCE FOR CHANGES IN INFLUENT, RECYCLE AND WASTE FLOW RATES

Thomas Vereș-Dănciuț[1,*], Vasile-Mircea Cristea[1], Adina-Lucreția Miclăuș[1], Elisabeta-Cristina Timiș[1]

[1]Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Cluj-Napoca, Romania

Abstract: *The study presents the assessment of the Pumping Energy (PE), Effluent Quality (EQ) and GreenHouse Gas (GHG) emissions performance indices of the Waste Water Treatment Plant (WWTP) in different operating scenarios. These scenarios consist in changing influent flowrate, return sludge flow rate, internal recycle flow rate and waste sludge waste flow rate. The pumping energy is most affected by modifications to the return sludge flow rate. Effluent quality and GHG emissions are most affected by the influent flow rate changes.*

Key words: wastewater treatment modelling, performance indices, sensitivity to plant flow rates

Introduction: The wastewater treatment industry is facing growing challenges due to world population increase and urbanization. Several quality indices have been established in order to monitor plant performance. This sensitivity study monitors the influence of several operating variables, such as influent flowrate, return sludge flow rate, internal recycle flow rate and waste sludge waste flow rate, on the plant performance indices.

Experimental and/or Modelling: *Model*: The simulations were carried out using the modified Benchmark Simulation Model No. 1 (BSM1) [1], calibrated for the anaerobic-anoxic-oxic configuration of the municipal WWTP serving as case study. The monitored indices are Pumping Energy, Effluent Quality and GHG emissions [2]. *Simulation Scenarios*: The studied scenarios consisted in the step modifications of the main mentioned WWTP flow rates. Each of these flow rates were modified independently, being increased and decreased by ±5% steps, up to ±20%. Simulation results were collected and analyzed.

Results and discussions: From the whole set of simulations, results obtained for the increase of the return sludge flow rate are presented in Figure 1.

Table 1 showcases the performance indices results, as percentage differences relative to the reference scenario, for a 10% increase in influent flow rate, return sludge flow rate, internal recycle flow rate and waste sludge flow rate.

* Corresponding author: thomas.veres@stud.ubbcluj.ro

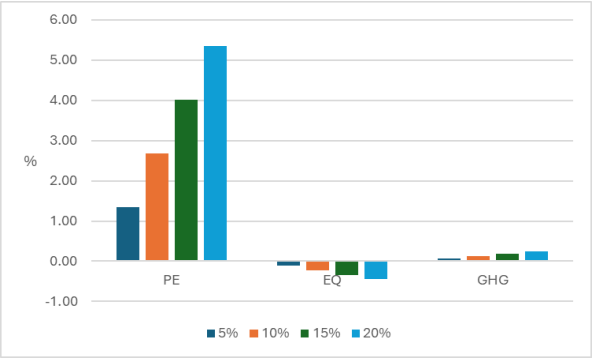


Figure. 1 Simulation results for increased return sludge flow rate, as percentage differences relative to the reference scenario

Table 1 ***Simulation results for a 10% increase in all studied flow rates, as percentage differences relative to the reference scenario***

	Pumping Energy	Effluent quality	GHG Emissions
Increased Influent Flow Rate	0.00	3.97	2.43
Increased Return Sludge Flow Rate	2.68	-0.23	0.13
Increased Internal Recycle Flow Rate	0.16	-0.48	0.01
Increased Sludge Waste Flow Rate	0.01	-0.29	0.00

Conclusions: The pumping energy is most affected by modifications to the return sludge flow rate. Effluent quality and GHG emissions are most affected by the influent flow rate. The results of the study reveal which of the main flows rates associated to the WWTP operation have larger impact on the plant performance indices and offers a valuable insight for the design of the WWTP control and decision support system.

Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0666, within PNCDI IV.

References:

[1] Alex J., Benedetti L., Copp J., Gernaey K. V., Jeppson U., Nopens I., Pons M.-N., Steyer J. P., Vanrolleghem P., *Benchmark Simulation Model no. 1 (BSM1)*, 2018 http://iwa-mia.org/wp-content/uploads/2019/04/BSM_TG_Tech_Report_no_1_BSM1_General_Description.pdf, 24.10.2025.

[2] Gernaey K. V., Jeppsson U., Vanrolleghem P. A., Copp J. B., *Benchmarking of Control Strategies for Wastewater Treatment Plants*, Scientific and Technical Report Series No. 23, 2014.

SA-OP11 DEEP LEARNING-BASED APPROACH: A VERSATILE DECODER FOR BUBBLE FLOW IMAGE ANALYSIS

T. N. Ngo[1,*], C. Vial[1], A. Essid[1], J. S. Guez[1], T. Château[1]

[1]Université Clermont Auvergne, Clermont Auvergne INP, CNRS,

Institut Pascal, 63000 Clermont-Ferrand, France

Abstract: *A lightweight model for the detection of gas bubbles in bubble flow images, allowed to reach over 90% of mAP50 while maintaining an inference speed of 111,94 FPS.*
Key words: Two-phase bubble size distribution, object detection, deep learning,

Introduction: In gas-liquid mass transfer research [1], understanding bubble flow inside reactors is essential. Key parameters such as volumetric transfer coefficient, interfacial surface area, and Sauter mean diameter [2] are closely related to bubble detection. To meet these demands, a deep learning detector that enables identification of bubbles in each scene at a high speed was explored.

Experiments: *Acquisition:* Bubble images were captured at a laboratory scale bubble column reactor. Distilled water was injected from the top while the gas was entering counterflow, using a high-speed camera at various pressures and flow rates. *Dataset:* 1,083 image patches containing 40,537 bubbles were used for training and validation. *Training:* YOLOv11-nano [3] was adopted with an upscaling factor of 4 during training to ensure the detection of every tiny bubble.

Results and discussions: Using the lightest model, a challenge mAP of 50.8% and a mAP50 of 91.6% at 111.94 FPS was achieved. Figure 1 (left) shows that the detector localizes nearly all bubbles in a cropped region with high precision bounding boxes, even when they overlap. By relating the predicted box width and height to the major and minor axes of bubble (ellipsoidal form), and then computing an equivalent diameter, the bubble size distribution was estimated immediately after detection. Nonetheless, some strongly overlapping bubbles remained false negative (highlighted in blue), resulting in the inaccuracy of the bounding boxes (yellow). Orientation of bubbles was not yet considered.

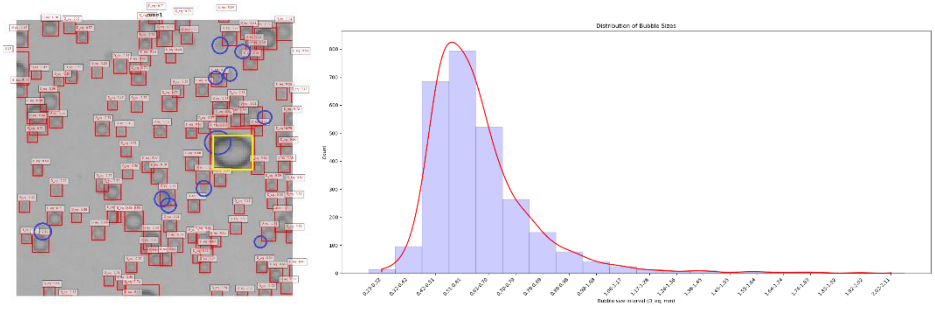


Fig. 1: Left – a zoomed qualitative view; right – the bubble size distribution in mm.

* Corresponding author: trong_nghia.ngo@doctorant.uca.fr

Conclusions: Future work will refine bubble size estimation by integrating bubble orientation, thereby improving the precision of the size distribution.

References:

[1] M. Keramati et.al. Intensification of ex-situ biomethanation in a bubble column bioreactor by addition of colonized biochips. Bioresource Technology Reports, 27 :101938, 2024.

[2] B. Sanogo et.al. Exploring the impact of proteins and surfactants on oxygen mass transfer in gas-liquid bioreactors: an experimental investigation. Chemical Engineering Science, page 121146, December 2024.

[3] G. Jocher et .al. Ultralytics YOLO11, 2024. https://github.com/ultralytics/ultralytics.

SA-OP12 DYNAMIC ADSORPTION BEHAVIOR OF VOLATILE ORGANIC COMPOUNDS ON A REGENERATIVE CELLULOSE-SILICA GEL COMPOSITE – EXPERIMENTAL INVESTIGATION AND MATHEMATICAL MODELLING

Ionuț-Alexandru Popa[1], Iuliana Mihaela Deleanu[1], Oana Cristina Pârvulescu[1], Timur-Vasile Chiș[2], Tănase Dobre[1 3] *

[1] University POLITEHNICA Bucharest

[2] University of Oil and Gas of Ploiesti

[3] Romanian Chemical Engineering Society

Abstract: *Building of a breakthrough curve for the adsorption of one volatile organic compounds from air onto a cellulose-silica gel composite adsorbent and use of breakthrough curve to identify the external particle mass transfer coefficient and of interphase equilibrium repartition coefficient*
Key words: Volatile Organic Compounds, Adsorption Dynamics, Adsorption Experimental Investigation, Mathematical Modelling, Breakthrough Curves, Mass Transfer Coefficients

Introduction: Volatile organic compounds (VOC) constitute a wide class of organic chemicals with high vapour pressure and low water solubility, many of which are used as solvents or emitted as process-related fugitive emissions; they are important both as pollutants and as occupational hazards in manufacturing environments. Regulatory and health concerns regarding VOC have motivated extensive efforts to reduce emissions at source and to treat exhaust streams prior to release to the atmosphere [1]. The automotive industry is a major emitter of process-related VOC, principally from paint shops and solvent-based surface treatments where coatings, thinners and cleaning agents are widely used. Workplace exposure and factory-level emissions in vehicle manufacturing and repair have been repeatedly documented, highlighting the need for robust abatement and monitoring strategies in both production and maintenance facilities [2],[3].

Experimental Investigation: The laboratory setup has consisted of two main sections, i.e. a gas-VOC vapor mixture preparation section and an adsorption-heating section. With registered experimental data it can builds the adsorbent saturation curve. It represent the time evolution of concentration of retained COV (qi) in the fixed bed at time τi. At a given τi the value of qi becomes from relation (1) where mi is the bed registered mass and m0 is the bed mass at experiment beginning.

$$q_i = \frac{m_i - m_0}{m_0} \qquad (1)$$

A Langmuir monolayer adsorption of VOC molecules onto the surface of cellulose-silica gel composite particles was taking into account in order to describe

* Corresponding author: tanase.dobre@upb.ro

the chemisorption equilibrium. When the bed is saturates at a fixed working temperature (t) the VOC concentration in the adsorbent, named q_∞ (g/g), is in equilibrium with the VOC concentration from gaseous phase noted as , $c_\infty = c_0$ (g/cm^3) where c_0 is the VOC concentration in gas that input in adsorption column. The values of c_∞ were calculated according to Eq. (2) where $m_{ev} = m_{0b} - m_{finb}$ (g) represents VOC mass picked-up by the carrier gas (the difference between mass of bubbler with COV at input and at finish of experiment) , $\tau_{fin} = \tau_{sat} + 200$ (s) is final operation time, and G_V (l/h) represent he gas volumetric flow rate (in the second part of relation (2) w is gas fictive velocity in m/s)

$$c_\infty = c_0 = \frac{3600\, m_{ev}}{G_V \tau_{fin}} = \frac{m_{0b} - m_{finb}}{w \tau_{fin} \dfrac{\pi d_c^{\,2}}{4}} \qquad (2)$$

Mathematical model: The dynamics of VOC species adsorption from air stream onto fixed bed cellulose-silica gel composite material and M/BC is been predicted by a model including transport and mass balance of VOC species. This model has been based on the following simplifying assumptions: i) flow pattern of gas phase along the column is axially dispersed plug flow, ii) phases densities are invariant due to process operating at constant temperature, iii) pressure drop across the bed is negligible and radial dispersion go to perfect mixing for this direction, iv) characteristic surface reaction of chemisorption is the process rate-limiting step, v) a monolayer adsorption of VOC molecules occurs onto the surface of adsorbentsites , according to the Langmuir model, vi) overall adsorption rate of species is equal to the difference between forward reaction (adsorption) rate, R_a, and backward reaction (desorption) rate, R_d, vii) R_a varies linearly with free surface site ratio, 1-q/Q, and species concentration in gas phase, *i.e.*, $R_{ai} = k_a \varepsilon_b (1-q/Q)c$, where k_a (s^{-1}) is adsorption rate constant and Q (g/g) maximum adsorption capacity at monolayer level and viii) R_d varies linearly with species adsorption capacity, q *i.e.*, $R_d = k_d \rho_b q$, d.

Results and discussions: Experimental investigations were carried out using cellulose–silica gel composite particles characterized by three distinct particle size ranges: large, small, and mixed distributions. The intermediate size fraction, corresponding to approximately half the mean diameter of the largest particles, was selected for detailed analysis to assess the influence of particle dimensions on column performance and mass transfer behavior.

Minor deviations at higher concentrations may be attributed to non-ideal flow effects or localized mass transfer limitations. Such consistency demonstrates that the assumptions regarding external film resistance and adsorption equilibrium are valid for the studied system.

Table 1. The constants k_{11} and k_{21} obtained after integration

Experiment Number	Particle Size (mm x mm)	CH_2Cl_2 Mass (g)	Temperature (°C)	Air Flow (L/h)	Column Layer Height (cm)	k_{11}	K_{21}
1	7 x 7	48,15	40	30	11,5	$2,35*10^{-4}$	$400*10^{-6}$
2	7 x 7	25,5	40	15	11,5	$1,55*10^{-4}$	$400*10^{-6}$
3	7 x 7	55,4	20	30	11,5	$2,85*10^{-4}$	$40*10^{-6}$
4	7 x 7	29,55	20	15	11,5	$2,25*10^{-4}$	$400*10^{-6}$
5	3,5 x 3,5	37,75	20	30	9,5	$5*10^{-4}$	$400*10^{-6}$
6	3,5 x 3,5	38,5	20	15	9,5	$3*10^{-4}$	$40*10^{-6}$
7	3,5 x 3,5	38,8	40	30	9,5	$3,75*10^{-4}$	$400*10^{-6}$
8	3,5 x 3,5	32,15	40	15	9,5	$2,45*10^{-4}$	$400*10^{-6}$
9	5,25 x 5,25	31,3	30	22,5	10,5	$2,85*10^{-4}$	$400*10^{-6}$
10	5,25 x 5,25	28	30	22,5	10,5	$2,65*10^{-4}$	$400*10^{-6}$
11	5,25 x 5,25	43,6	30	22,5	10,5	$3,85*10^{-4}$	$400*10^{-6}$
12	5,25 x 5,25	35,65	30	22,5	10,5	$3,55*10^{-4}$	$400*10^{-6}$

Therefore, the developed model can be confidently employed for process design, optimization, and scale-up of the adsorption unit.

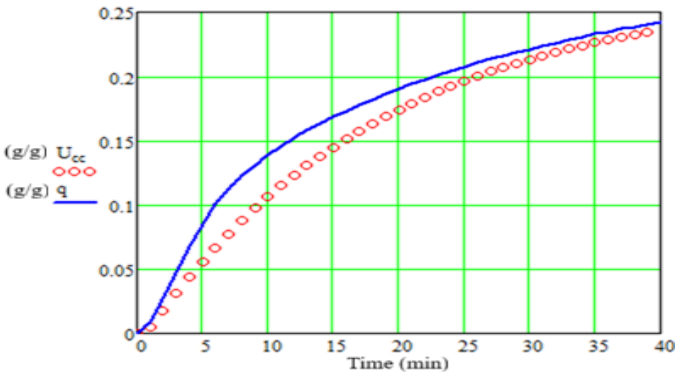


Figure 1. Graphical representation of the proposed integrated theoretical model versus experimental data

The comparison between curves highlights the influence of external mass transfer resistance and adsorption kinetics on the overall process dynamics. The observed shapes and slopes of the curves indicate a system predominantly controlled. These results demonstrate a good agreement between the numerical model and the expected theoretical behavior.

References

[1] U.S. Environmental Protection Agency. *What are volatile organic compounds (VOCs)?* EPA Indoor Air Quality (IAQ) — VOCs. (accessed Octomber 2025)

[2] Song, M.-Y., et al. *Species and characteristics of volatile organic compounds from industrial and indoor sources.* Sci. Rep. 11, 2021

[3] Ghobakhloo, S., et al. *Exposure to Volatile Organic Compounds in Paint Operations: Occupational Assessment and Health Implications.* Int. J. Environ. Res. Public Health 20, 2023

[4] Shi, R.-J., et al. *Multifunctional Cellulose and Cellulose-Based (Nano)materials: Applications in Adsorption and Beyond.* Materials, 2022

SA-OP13 QUANTITATIVE VISUALIZATION OF HYDROGEN MASS TRANSFER IN AQUEOUS MEDIA

Blandine Tauleigne[1,*], Alain Marcati[1], Christophe Vial[1]

[1]Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, F-63000 Clermont-Ferrand, France

Abstract: *A new colorimetric technique based on a hydrogen-sensitive redox dye was investigated for the quantitative visualization of hydrogen mass transfer. The method employs sodium anthraquinone-2-sulfonate (AQ2S) as a color indicator and palladium chloride ($PdCl_2$) as a catalyst in an alkaline medium, as previously reported for hydrogen detection. The influence of catalyst concentration was examined to ensure that the colorimetric reaction proceeds faster than mass transfer without altering it, for a real-time mass transfer visualization. Excessive $PdCl_2$ concentrations generated visible particles that interfered with observation, leading to the selection of an optimal concentration for subsequent tests. The color intensity was correlated with the amount of hydrogen consumed, demonstrating the method's ability to reflect mass transfer phenomena. Ongoing modeling aims to relate color intensity to concentration as a function of liquid path length, enabling future single-bubble studies. Overall, the approach shows promising potential for quantitative visualization of hydrogen mass transfer, with sensitivity to be further assessed in single-bubble experiments.*

Key words: Hydrogen Visualization, Mass transfer, color intensity.

Introduction: In the context of the energy transition, hydrogen has attracted growing interest due to its potential applications. Emerging green processes involving hydrogen often highlight its mass transfer as a major limiting step. Understanding this limitation requires an investigation of the gas–liquid interface and the influence of operating parameters. Given that hydrogen remains far less studied than other gases such as oxygen, addressing this knowledge gap is essential for optimizing hydrogen-based technologies.

Experimental: The colorimetric method investigated employs sodium anthraquinone-2-sulfonate (AQ2S, $1{,}8.10^{-5}$—$3{,}6.10^{-4}$ mol/L) as a hydrogen-sensitive redox indicator and palladium (II) chloride ($PdCl_2$, $1{,}8.10^{-7}$—$1{,}8.10^{-3}$ mol/L) as a catalyst in sodium hydroxide-water solution [1]. The experimental setup consists of a steel reactor with an optical path length of 150 mm, equipped with H_2 and pH/ORP sensors, and allowing video recording and absorbance monitoring. Since the reduced form of AQ2S is highly sensitive to oxygen, experiments had to be conducted under an inert gas atmosphere.

Results and discussions: Preliminary experiments examined the effect of catalyst concentration on the colorimetric reaction rate. The catalyst affects the reaction rate, which must exceed hydrogen mass transfer to enable real-time monitoring, without influencing the transfer itself. Within the studied concentration range, no enhancement of mass transfer was observed, though low $PdCl_2$ solubility posed

* Corresponding author: blandine.tauleigne@doctorant.uca.fr

visualization challenges. A minimum effective concentration was identified, and an optimal concentration was selected for subsequent experiments.
The intensity of the color change was found to depend on both the optical path length and the amount of reacted AQ2S, which directly correlates hydrogen consumption. To quantify this relationship, dedicated tests with shorter path lengths (2,5—40 mm) were conducted. Figure 1 shows the color change during one of these tests. Ongoing modeling efforts aim to enable future single-bubble studies.

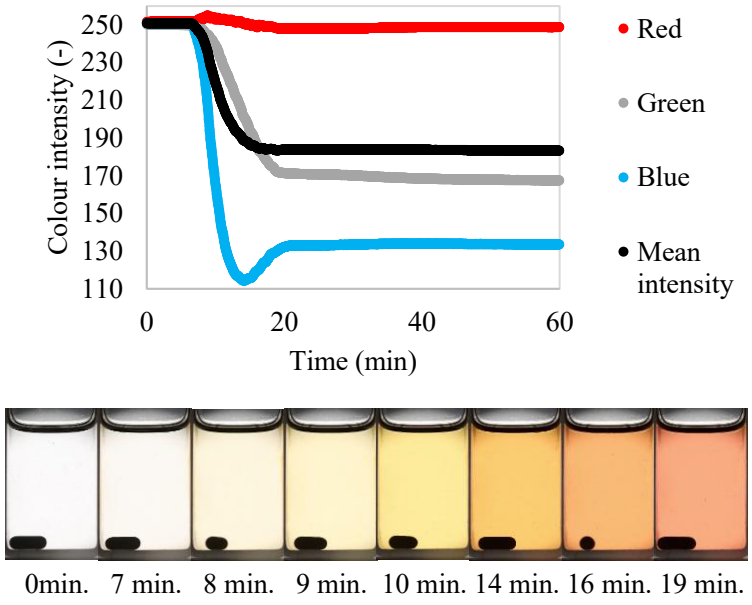


Fig. 1 Graphical visualization of the RGB color evolution and corresponding color change for an optical path length of 10mm, with AQ2S and $PdCl_2$ concentrations of $1{,}8.10^{-4}$ mol/L.

Conclusions: This method shows promising potential for quantitative visualization of hydrogen mass transfer, with sensitivity to be assessed in single-bubble studies.

References:

[1] Silverman L. and Bradshaw W., "Determination of small quantities of hydrogen in the inert gases," *Analytica Chimica Acta*, vol. 15, pp. 31–42, July 1956, doi: 10.1016/0003-2670(56)80007-X.

BOOK OF ABSTRACTS

SICHEM – 2025

A – Chemical and biochemical engineering (CBE)

3. Poster presentations

SA-P01 TRANSPARENT AI MODELS FOR CHEMICAL PROCESS DIAGNOSTICS: INSIGHTS FROM ONER AND JRIP

Andrei Coman[1,*], Silvia Curteanu[2]

[1]"Cristofor Simionescu" Faculty of Chemical Engineering and Environmental Protection, "Gheorghe Asachi" Technical University of Iași, 73 Dimitrie Mangeron Blvd., Iași, Romania

[2]"Cristofor Simionescu" Faculty of Chemical Engineering and Environmental Protection, "Gheorghe Asachi" Technical University of Iași, 73 Dimitrie Mangeron Blvd., Iași, Romania

Abstract: *This paper investigates the use of Explainable Artificial Intelligence (XAI) in chemical engineering, focusing on rule-based methods that combine interpretability with operational value. Two case studies were developed on synthetic datasets representative of industrial processes. The first applies the OneR algorithm to water quality monitoring, while the second uses JRip for industrial emissions classification. Results highlight how these interpretable models can support diagnostics, process optimization, and compliance with regulatory requirements.*

Keywords: Explainable Artificial Intelligence; OneR; JRip; Chemical Engineering; Process Monitoring; Industrial Emissions

Introduction: Modern chemical processes require not only accurate predictions but also explanations that can be directly validated by engineers. In safety-critical environments, decisions must be justified through clear and auditable logic. Rule-based algorithms such as OneR and JRip address this challenge by generating transparent models in the form of simple rules or compact rule sets [1]. Their outputs can be immediately interpreted, integrated into operational procedures, and verified against domain knowledge. This work explores how these two algorithms can provide practical value for process monitoring and emissions control in chemical engineering [2,3].

Experimental and Modelling: Two case studies were developed. Case Study 1 applied OneR to classify water quality based on four input variables: pH, conductivity, TOC, and temperature. The output was the water quality class, labeled either Compliant or Non-compliant. The dataset included observations representative of industrial cooling or treatment processes. Case Study 2 used JRip to classify industrial emissions. Six input variables were considered: combustion temperature, residual oxygen, gas flow rate, NOx, SO_2, and VOC (COV_mg/m³). The output variable was emissions compliance, defined as either Compliant or Exceedance based on regulatory thresholds. The dataset contained 200 hourly observations from a petrochemical scenario. Both models were trained and validated using 10-fold cross-validation to assess predictive accuracy and rule interpretability [3,4].

Results and discussions: In Case Study 1, OneR generated a simple one-rule model where pH emerged as the primary predictor of water quality. Figure 1 shows the distribution of pH values by class, clearly illustrating how deviations from the

* Corresponding author: andreicoman22@gmail.com

acceptable range separate compliant from non-compliant cases. This transparent structure facilitates immediate validation by process experts and allows straightforward integration into monitoring routines. In Case Study 2, JRip identified VOC concentration as the key factor for emissions classification. Figure 2 presents the average VOC levels for each class, confirming that exceedance cases are strongly associated with higher VOC values. The resulting rule set was compact and interpretable, achieving high accuracy while providing auditable criteria directly applicable to environmental compliance. Together, the two case studies demonstrate how OneR emphasizes extreme simplicity and interpretability, while JRip offers robustness through multi-rule models that remain transparent. [2,4].

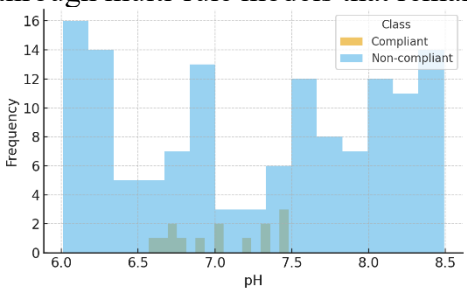


Fig. 1 Distribution of pH values by class (Compliant vs. Non-compliant) in the water quality dataset.

Fig. 2 Average VOC levels by class (Compliant vs. Exceedance) in the industrial emissions dataset.

Conclusions: OneR highlights the value of simplicity in scenarios where a single discriminant factor can provide fast and transparent classification. JRip, in contrast, delivers higher robustness through multi-rule models, ensuring accuracy while keeping interpretability. Taken together, these findings show that rule-based XAI methods can support diagnostics, predictive maintenance, and compliance with environmental standards in chemical engineering.

References:

[1] Guidotti, R., Monreale, A., Ruggieri, S., Turini, F., Giannotti, F., & Pedreschi, D. (2018). A Survey of Methods for Explaining Black Box Models. ACM Computing Surveys, 51(5), 93.

[2] Hara, S., & Hayashi, K. (2018). *Making Tree Ensembles Interpretable: A Bayesian Model Selection Approach*. Proc. AAAI Conference on Artificial Intelligence.

[3] Zhang, H., et al. (2020). *Interpretable Machine Learning for Industrial Process Data: Case Studies and Perspectives*. Computers & Chemical Engineering, 139, 106904.

[4] Carvalho, D. V., Pereira, E. M., & Cardoso, J. S. (2019). *Machine learning interpretability: A survey on methods and metrics*. Electronics, 8(8), 832.

SA-P02 EXPLAINABLE AI METHODS FOR DIAGNOSTICS AND OPTIMIZATION IN CHEMICAL PROCESSES: CASE STUDIES WITH J48, LINEAR REGRESSION, M5P AND M5RULES

Dumitriana-Roberta-Marina Brănescu[1,*], Silvia Curteanu[1]

[1]"Cristofor Simionescu" Faculty of Chemical Engineering and Environmental Protection, "Gheorghe Asachi" Technical University of Iași, 73 Dimitrie Mangeron Blvd., Iași, Romania

Abstract: *In this work, the focus is placed on the integration of interpretable machine learning models into chemical process analysis, with the aim of balancing predictive performance and transparency. Two representative case studies are presented. The first explores the classification of pump operating states using J48 decision trees. The second addresses a distillation column scenario where M5P and M5Rules are applied alongside Linear Regression to capture nonlinear dynamics through piecewise models and explicit rules. The findings emphasize the strengths and limitations of each method and demonstrate how interpretable approaches can transform data-driven models into practical decision-support tools for chemical engineers.*
Key words: Explainable Artificial Intelligence; Chemical Engineering; J48; Linear Regression; M5P; M5Rules; Process Optimization

Introduction: The digitalization of the chemical industry, accelerated by Industry 4.0, relies on advanced data-driven models for monitoring, optimization, and fault detection. While AI systems improve performance, black-box behavior limits trust and regulatory compliance. Explainable AI (XAI) methods respond to this challenge by enabling transparent and auditable decision making [1]. Recent studies emphasize the importance of interpretable models in safety-critical domains, including chemical engineering [2,3].

Experimental and Modelling: Two datasets representative of industrial processes were analyzed in this work. The first case study focused on pump diagnostics. The dataset consisted of observations, each described by three input variables: temperature, vibration, and pressure, with the output representing the operating state, either "OK" or "Failure." The second case study addressed the optimization of a distillation column. In this scenario, the dataset included several process variables as inputs, namely reflux ratio, top pressure, feed temperature, light-key fraction, column load, ambient temperature, and purity. Models tested included J48 decision tree, Linear Regression, and the model tree algorithms M5P and M5Rules [3,4].

Results and discussions: For Case Study 1, J48 achieved approximately 98% classification accuracy, generating simple and interpretable rules based on vibration thresholds (≤0.82 g → "OK"; >0.82 g → "Failure"). As shown in Figure 1, these rules align directly with the distribution of the pump operating states, making them highly suitable for integration into monitoring procedures.

For Case Study 2, Linear Regression explained around 96% of the variance but proved insufficient in capturing the nonlinear regimes of the distillation process. Figure 2 illustrates this nonlinear relationship between reflux ratio and specific energy consumption, which was more accurately modeled using M5P and M5Rules. These methods significantly

* Corresponding author: roberta.branescu@gmail.com

improved predictive performance ($R^2 \approx 0.995$, RMSE ≈ 8.2 kWh/t) by partitioning the input space into distinct regions with explicit local equations or rules. Their outputs provided both high numerical accuracy and human-readable explanations, making them practical tools for process optimization and compliance audits.

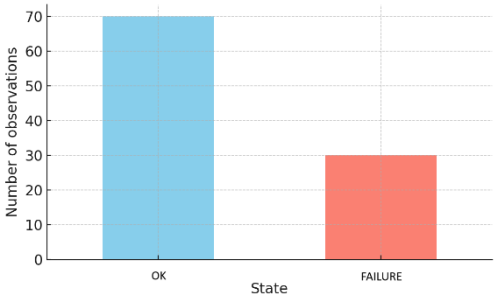


Fig. 1 Distribution of pump operating states (OK vs. Failure)

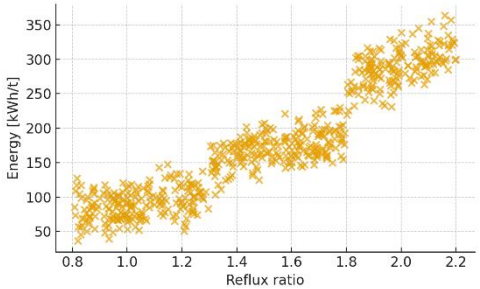


Fig. 2 Nonlinear relationship between reflux ratio and energy consumption in the distillation column.

Conclusions: Linear Regression provides a transparent baseline but remains limited when applied to nonlinear chemical processes. J48 emerges as a practical solution for equipment diagnostics, combining high accuracy with simple operational rules that can be directly implemented in monitoring systems. M5P and M5Rules strike a better balance between predictive power and interpretability, offering piecewise equations and human-readable rules that capture complex dynamics while remaining accessible to engineers. Taken together, these methods confirm the importance of Explainable AI for sustainable and safe chemical engineering. Beyond their academic value, interpretable models provide transparency, traceability, and compliance support, making them highly relevant in industrial environments where both performance and accountability are critical.

References:

[1] Doshi-Velez, F., & Kim, B. (2017). Towards a rigorous science of interpretable machine learning. arXiv preprint arXiv:1702.08608.; **[2]** Molnar, C. (2022). Interpretable Machine Learning. 2nd ed. Available: https://christophm.github.io/interpretable-ml-book/; **[3]** Ribeiro, M.T., Singh, S., & Guestrin, C. (2016). "Why Should I Trust You?" Explaining the Predictions of Any Classifier. Proc. KDD. Available: https://dl.acm.org/doi/10.1145/2939672.2939778; **[4]** Lundberg, S.M., & Lee, S.I. (2017). A Unified Approach to Interpreting Model Predictions. Advances in Neural Information Processing Systems.

SA-P03 PRE-BIOREACTOR ASSESSMENT OF CULTURE MEDIA FOR CAROTENOID PRODUCTION BY *RHODOTORULA RUBRA* ICCF 220

Vlad-Iulian Chelmuș[1], Teodora Moraru[1,2], Alina Mihalcea[2], Camelia Ungureanu[1*]

[1] National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, 313 Splaiul Independenței, 060042 Bucharest, Romania.

[2] Cantacuzino National Institute of Research and Development for Microbiology and Immunology, 103 Splaiul Independenței, 050096 Bucharest, Romania.

Abstract: *The optimization of culture media is essential for improving the biosynthesis of microbial metabolites, particularly carotenoid pigments of industrial interest. This study assessed the effect of various carbon and nitrogen sources on the growth and pigmentogenic activity of Rhodotorula rubra ICCF 220. Four media with different C/N ratios were tested under controlled conditions, and growth parameters were monitored by optical density, cell number, pH, and soluble solids content. The results highlight the importance of medium composition for maximizing pigment yield and biomass accumulation.*

Key words: Rhodotorula rubra ICCF 220; carotenoid pigments; culture media optimization; carbon and nitrogen sources; microbial growth; bioprocessing

Introduction: Carotenoid pigments produced by yeasts of the genus *Rhodotorula* are of growing biotechnological interest due to their antioxidant and coloring properties. The composition of the culture medium, along with temperature, pH, aeration rate, and illumination, represents a key factor influencing growth and metabolite synthesis. This work focuses on identifying suitable combinations of carbon and nitrogen sources for improving biomass formation and carotenoid accumulation in *R. rubra* ICCF 220 [1,2].

Experimental: The yeast strain *Rhodotorula rubra* ICCF 220 was maintained on Sabouraud agar and used to inoculate four liquid media differing in carbon and nitrogen sources: MS3 (glucose/nitrate), M1 (glycerol/sulfate), M2 (malt extract/glycerol), and M3 (sucrose/organic nitrogen). Cultivations were carried out in 500 mL Erlenmeyer flasks containing 100 mL of medium, at 30 °C and 150 rpm for 144 h. Samples were taken every 24 h for the optical density at 600 nm (OD_{600}), pH, cell counts, and soluble solids (SU %). Biomass was separated by centrifugation, washed, and used for carotenoid extraction with a hexane–methanol biphasic system.

Results and discussions: The yeast showed distinct growth profiles depending on the carbon and nitrogen sources. The glucose/nitrate medium (MS3) yielded the highest biomass and pigment content, with OD_{600} values about 14 % higher than in glycerol/sulfate medium (M1). Media M2 and M3 led to slower growth and lower pigment accumulation, reflecting limited nutrient assimilation. Refractometric SU % decreased as biomass increased, confirming nutrient consumption. During

* Corresponding author: camelia.ungureanu@upb.ro; ungureanucamelia@gmail.com

cultivation, pH decreased gradually, reaching 2–3 after 144 h in MS3, consistent with active metabolism. These findings confirm that glucose and nitrate favor pigment biosynthesis and represent optimal conditions for further bioreactor studies.

Conclusions: Medium composition markedly affects carotenoid pigment production in *R. rubra* ICCF 220. The MS3 medium (glucose/nitrate) ensured the best growth and pigment accumulation, serving as reference for pre-bioreactor optimization.

References:

[1] Li Z., Li C., Cheng P., Yu G., *Rhodotorula mucilaginosa* — alternative sources of natural carotenoids, lipids, and enzymes for industrial use, *Heliyon*, 8, 11, (2022), e11505. https://doi.org/10.1016/j.heliyon.2022.e11505

[2] Fonseca R. S. K., Lotas K. M., Cortez A. C. A., Fernandes F. S., Souza É. S., Dufossé L., de Souza J. V. B., Exploration of carotenoid-producing *Rhodotorula* yeasts from Amazonian substrates for sustainable biotechnology applications, *Current Research in Microbial Sciences*, 8, (2025), 100373. https://doi.org/10.1016/j.crmicr.2025.100373

SA-P04 EXPERIMENTAL STUDY ON THE INFRARED DRYING OF USED COFFEE GROUNDS

Laurențiu-Constantin Mihailă, Gabriela Lisa[1,*]

[1]"Gheorghe Asachi" Technical University of Iasi-Romania, Faculty of Chemical Engineering and Environmental Protection "Cristofor Simionescu", 73 prof. dr. doc. D. Mangeron street, 700050, Iasi, Romania

Abstract: *Used coffee grounds, with energy potential, can be converted into biodiesel, bioethanol, bio-oil, or pellets. Efficient drying, keeping moisture below 10%, is essential but energy-intensive. This study investigated infrared drying, focusing on kinetics and process optimization. Experiments with a Mettler Toledo HG63 moisture analyzer at 50, 60, and 70ºC on ~23 g samples showed drying speed increases with temperature, reducing drying time from 470 min at 50ºC to 220 min at 70ºC. Results aligned with literature, demonstrating the method's feasibility.*
Key words: Used coffee grounds, Drying, Kinetic study

Introduction: Used coffee grounds, with energy potential, can be converted into biodiesel, bioethanol, bio-oil, or pellets. Drying, essential for their use as green energy, requires significant energy (~5 MJ/kg of water in convective dryers) and must reduce moisture content below 10% to ensure storage and prevent microbial growth. Infrared drying accelerates the process through direct heating, although thick layers may lead to uneven drying. This study investigated the drying of coffee grounds using this method to determine drying rates, model the process, and optimize its performance.

Experimental: The kinetic study of the used coffee grounds drying process was conducted using a Mettler Toledo HG63 halogen moisture analyzer. The mass of the samples subjected to drying in the analyzer was 22.769 ± 1.056 g. Samples were evenly distributed on the instrument's tray to ensure a uniform coffee grounds layer height. Experimental determinations were carried out at temperatures of 50, 60 and 70 ºC.

Results and discussions: Based on the experimental measurements, the moisture content of the material (MR) was calculated using the following equation:

$$MR = \frac{M(t) - M_e}{M_0 - M_e} \quad (1)$$

in which M_0 represents the initial moisture content of the used coffee grounds, M_e is the equilibrium moisture content determined from the drying curves at the point when the sample mass no longer changes with time, and M(t) is the moisture content of the sample at any given time. Additionally, the drying rate, expressed in kg/m²·s, was determined. The drying curves obtained under isothermal conditions at 50 ºC, 60 ºC and 70 ºC, representing the variation of moisture content in the material as a function of drying time, are presented comparatively in Figure 1. At 50 ºC, complete

* Corresponding author: gabriela.lisa@academic.tuiasi.ro

drying of the coffee grounds was achieved in 470 minutes, while at 70 ºC it was completed in 220 minutes. Taking into account the tray surface area used for the experimental measurements in the Mettler Toledo HG63 halogen moisture analyzer, namely 0.00694 m², the drying rate at different temperatures was calculated and expressed in kg/m²·s. The results are graphically presented in Figure 2 as a function of moisture content u, expressed in kg of moisture per kg of initial sample. The drying rate increases with increasing temperature.

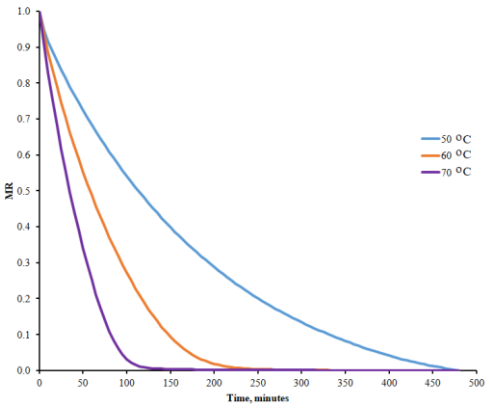


Fig. 1 MR as a function of time

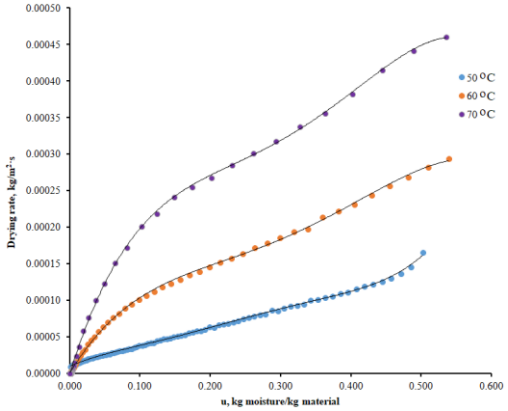


Fig. 2 Drying rate as a function of moisture content

The obtained results were compared with those reported in a previous study in which drying was performed using a Mettler Toledo TGA-SDTA851ᵉ, simulating conditions in industrial tubular dryers [1]. A good agreement was observed; for example, at 70 ºC, the maximum moisture removal rate in the previous study was 0.00048 kg/m²·s, compared to 0.000459 kg/m²·s in the present study.

Conclusions: Infrared drying of coffee grounds accelerates the process by increasing temperature, with drying rate directly proportional to temperature and inversely proportional to layer thickness, enabling reduction of moisture below 10% for safe storage and prevention of biological degradation; experimental data align well with previous studies, supporting the method's applicability for pilot- or industrial-scale optimization and confirming the potential of coffee grounds as a renewable energy resource, justifying further research on efficient drying and energy valorization.

References:

[1] Bejenari V., Lisa C., Cernatescu C., Mamaliga I., Lisa G., Isothermal Drying Kinetic Study of Spent Coffee Grounds Using Thermogravimetric Analysis, Int. J. Chem. Eng., (2022), Article ID 2312147.

SA-P05 RECOVERY OF USED COOKING OILS: EVALUATION OF PHYSICO-CHEMICAL PROPERTIES AND ANALYSIS OF THE FILTRATION PROCESS

Paula Rusu[1], Cătălin Lisa[1,*]

[1]"Gheorghe Asachi" Technical University of Iasi-Romania, Faculty of Chemical Engineering and Environmental Protection "Cristofor Simionescu", 73 prof. dr. doc. D. Mangeron street, 700050, Iasi, Romania

Abstract: *The study investigates the filtration process and physic-chemical characterization of used sunflower and palm oils, highlighting that filtration is an effective method for removing impurities, while the results confirm the potential of these waste oils as valuable resources for the production of biofuels and other sustainable products, thus contributing to the promotion of a circular economy.*
Key words: Used Cooking Oils, Filtration, Physico-chemical characterization

Introduction: The responsible management of used cooking oils represents a major challenge, as improper treatment can lead to water and soil pollution. However, these residues possess significant reuse potential, serving as sources for biofuels, chemical products, or biodegradable lubricants. Implementing efficient collection and recovery systems contributes to environmental protection, promotes the circular economy, and reduces dependence on fossil resources [1-3].

Experimental: This study examined the recovery of used sunflower and palm oils collected from household sources and the canteen of the "Gheorghe Asachi" Technical University of Iași. The oils were filtered using a Rover PULCINO unit with five plates, and their physic-chemical properties: density, refractive index, kinematic viscosity, and photometric color index were analyzed using standard laboratory equipment under controlled temperature conditions.

Results and discussions: The used cooking oils were subjected to a filtration process employing a Rover PULCINO device equipped with five plates and a capacity of 100–150 L/h to remove food residues. The characteristic filtration constants at constant pressure were determined as $k_v = 8\times10^{-4}$ m³/m² and $k_t = 1.7\times10^{-7}$ m²/s, values comparable to those reported in the literature [4]. In addition to the technological parameters of filtration, the physic-chemical properties of the fresh and used oils were analyzed, including density, refractive index, kinematic viscosity, surface tension, and photometric color index. The analysis revealed that density, refractive index, and surface tension remained largely unchanged after use, suggesting that these properties are less sensitive to thermal or oxidative degradation under typical cooking conditions. Conversely, both kinematic viscosity and photometric color index increased slightly for the used oils (Table 1), indicating the occurrence of thermal and oxidative degradation processes. The increase in viscosity can be attributed to polymerization and the formation of higher molecular

* Corresponding author: catalin.lisa@academic.tuiasi.ro

weight compounds during heating, while the darkening of the oils, reflected by the photometric color index, is consistent with the formation of oxidation products and Maillard reaction compounds.

Table 1

Kinematic viscosity and photometric color index for fresh and used cooking oil samples

Analyzed product	Photometric color index (PCI)	Kinematic viscosity (mm^2/s)	Temperature, °C
Sunflower oil	2.16±0.11	56.51±0.10	25
Used sunflower oil	2.51±0.10	58.33±0.05	25
Palm oil	1.53±0.12	34.86±0.01*	25, *50
Used palm oil	2.64±0.13	34.48±0.10*	25, *50

These findings demonstrate that while the filtration process effectively removes solid residues, the oils still undergo moderate changes in viscosity and color during use, highlighting the importance of monitoring these parameters for quality assessment in culinary and industrial applications.

Conclusions: The study concludes that filtration effectively removes food residues from used oils, while physicochemical characterization provides useful data for potential applications, such as biofuels, detergents, or lubricants. Monitoring viscosity and color is also important to assess thermal and oxidative degradation. Although filtration removes solids efficiently, moderate changes indicate that repeated reuse may affect food quality and increase degradation, so periodic evaluation is recommended to ensure safety and optimal reuse.

References:

[1] Miyuranga K.A.V., Arachchige U.S.P.R., Marso T.M.M., Samarakoon G., Biodiesel Production through the Transesterification of Waste Cooking Oil over Typical Heterogeneous Base or Acid Catalysts, *Catalysts*, 13, (2023), 546.

[2] Kulkarni M. G., Dalai A. K., Waste Cooking Oil An Economical Source for Biodiesel: A Review, *Ind. Eng. Chem. Res.*, 45, 9, (2006), 2901–2913.

[3] Sivriu, A.M., Jinescu G., Săpunaru (Țaga), O., Tîrpan, D.R., Koncsag, C.I., Pyrolysis of waste palm oil in presence of steam, *Rev. Chim. (Bucharest)*, 70, 2, (2019), 4175-4180.

[4] Lužaic T., Nedic G. K., Pezo L., Nikolovski B., Maksimovic Z., Romanic R. Implementation of Cellulose-Based Filtration Aids in Industrial Sunflower Oil Dewaxing (Winterization): Process Monitoring, Prediction, and Optimization, *Foods* 13, 2024, 2960.

SA-P06 A NUMERICAL OFFSHORE EXPLOSION MODELING IN NATURAL GAS DRILLING

Timur Chis[1*], Daniel Iancu[2], Lazar Avram[1], Calin Iorga[2]

[1]Oil and Gas Engineering Faculty, Petroleum-Gas University

[2]Ph.D. School, Petroleum-Gas University

Abstract: *The explosion of the Deepwater Horizon oil platform was one of the most serious accidents, leading to the loss of 5 million barrels (pollution of the Gulf of Mexico) and the disappearance of 11 people. That is why the description of a simulation model of an explosion on a marine platform makes the prevention activity useful, in the context of the increasing importance of the exploitation of the Black Sea. Through this material we simulated a possible explosion on a Romanian oil structure, in order to obtain the minimum data necessary to be quantified so that an incident does not occur.*

Key words: oil offshore, drilling platform, risk assessment, numerical models, oil rig explosion,

Introduction: Offshore activities, especially oil and gas exploration and exploitation, are risky ventures. Drilling a well and the risks it poses are not negligible. In addition, oil rigs are hazardous environments with heavy equipment, dangerous substances (flammable chemicals and gases), and remote locations from shore where weather and water conditions are unpredictable. In Romania, incidents of Offshore platforms it is at low level, because the strategy of working to Romanian Offshore Platforms is approve to the Life and Safety Management Authority Standards.

The entire process of risk management and the ALARP (As low as reasonably practicable) principle is based on a prerequisite of discernment. The principle assumes that most risks can be controlled, while only a tiny percentage of "remaining risk" needs to be tolerated - and should be managed cost-effectively.

This means that a significant amount of risk remains uncontrolled.

Experimental and/or Modelling: In what follows, we analyzed the explosion of the compressor on the offshore platform based on the phenomenon of natural gas dispersion in its ventilation system. This is cause to the more oil accidents. The extent of damage caused by releasing flammable gases is partly a function of cloud dispersion. If there is no immediate ignition, flammable vapors are dispersed through the structure's geometry (metal construction) and ventilation systems, and ignition may be delayed [1].

Ignition and explosion of the resulting vapor cloud (VCE) occur if the gas's flammability limits are met (based on gas composition) and an ignition source of sufficient energy is present [2].

Several factors, namely influence an explosion of a gas cloud [3]:

a. the probability of ignition increases with the size of the vapor cloud,

* Corresponding author: timur.chis@gmail.com

b. the effectiveness of the explosion and its impact is affected by the turbulent mixture of vapor and air,

c. the efficiency of the explosion depends on the location of the ignition sources,

d. the size of the explosion depends on the concentration of the explosive medium (gas cloud).

Results and discussions :

We analyzed a new relationship whose objective is to provide data on the opening value of the BOP (blowout preventer) according to the level of employee injury.

The multifactorial regression equation is of the form:

$$y=6,952-0,010\ x_1-3,434\ x_2+2,684\ x_3 \quad (1)$$

Where y is the opening of the BOP (% of exhaust pipe), x_1, x_2 and x_3 are the distances of fatal injury, hospitalization or minor burns (m)

Conclusion: In this material, we studied the accident on the Romanian oil platform, based to the:

a. risks assumed and not assumed following the drilling operation on the platform,

b. errors of the prevention and control mechanism,

c. eEffects of the oil platforms accident.

To observe how the BOP (blowout preventer) acted on the effects of the accident on the oil platform, we analyzed its closure.

References:

[[1] Elusakin, T., Shafiee, M., *Reliability analysis of subsea blowout preventers with condition-based maintenance using stochastic Petri nets, Journal of Loss Prevention in the Process Industries,* doi: https://doi.org/10.1016/j.jlp.2019.104026, 2020,

[2] Hopkins, P., Goodfellow, G., Ellis, R., Haswell, J., Jackson, N., *Pipeline risk assessment: new guidelines*, WTIA/APIA Welded Pipeline Symposium, Sydney, Australia, 2009.

[3] Sulaiman, D., Iancu, D., Al Jubori, H., *The current state of research on the dilation processes of productive reservoir rocks related to natural gas wells*, 75 Years of Energy and Performance in Education and Research 2023 Renewable Versus Fossil Fuels. Global Energy Perspectives, Ploiesti 9.11.2023, Book of abstracts, Editura Universității Petrol-Gaze din Ploiești, 2023, ISBN 978-973-719-887-7.

SA-P07 NUMERICAL MODELS APPLIED IN THE STUDY OF NATURAL GAS MOVEMENT IN UNDERGROUND DEPOSITS

Timur Chis[1]*, Ionut Lungu[2], Doru Barsan[1], Andrei Barbulescu[2]

[1]Oil and Gas Engineering Faculty, Petroleum-Gas University

[2]Ph.D. School, Petroleum-Gas University

Abstract: *Inside the cavity and the well, the gas does not behave adiabatically: it exchanges heat with the surrounding rock. It is not possible to accurately represent the cavity shape and heat exchanges in detail, partly because of imperfect knowledge of the geological environment and partly because a detailed three-dimensional numerical model would be far too time-consuming. This paper describted the storage of natural gas in salt underground deposits.*
Key words: oil salt, deposit, underground, numerical models.

Introduction: Numerical models thus help to optimize natural gas extraction processes and prevent technical and economic problems, providing a detailed understanding of the fluid dynamics inside the reservoirs.

Advantages are:

• The possibility of simulating complex and very diverse conditions, which cannot be studied directly

• The behavior of the deposit can also be modeled at different extraction and injection cycles, so that its management is much more accessible

• A result of the modeling processes is the reduction of deposit maintenance costs because they provide the critical parameters for the operation of the deposit.

Experimental and/or Modelling:

In the rock mass, the temperature field T_{roca} verifies the heat equation:

$$\rho_r \, c_p^r \frac{\partial T_{roc\check{a}}}{\partial t} + dic\,(-\lambda_{roc\check{a}} \nabla T_{roc\check{a}}) = 0 \qquad (1)$$

where :

ρ_r is the density of the rock,

c_p^r the specific heat capacity of the rock per unit mass, and λ rock is the thermal conductivity of the rock.

The temperature distribution is assumed to be spherically symmetric around the cavity. The rock mass surrounding the cavity is then discretized into spherical layers (Figure 1).

The cavity problem with the surrounding rock mass is solved as a one-dimensional coupled nonlinear problem.[1,2,3]

* Corresponding author: timur.chis@gmail.com

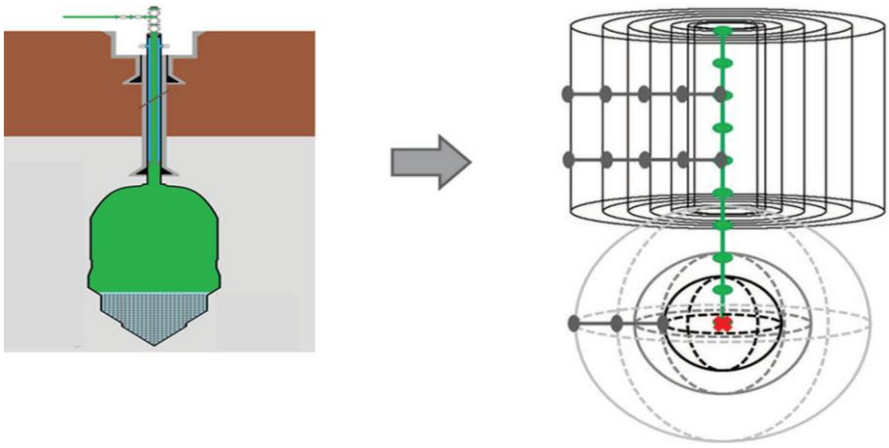


Fig. 1: Discretization of rock into spherical layers

Conclusion: This studied algorithm allows a robust and modular approach to take into account the heat exchange between the well and the rock mass.

Numerical models are mathematical simulations performed on a computer that allow the study of the behavior of complex physical systems, in this case, the movement of natural gas in an underground reservoir. They are based on solving differential equations that describe the relevant physical phenomena (such as fluid movement, heat transport, and the behavior of porous materials).

In the context of underground reservoirs, numerical models are used to simulate and predict:

- Gas flow under different geological and drilling conditions.
- Reservoir behavior during gas injection or extraction.
- Long-term thermal behavior and gas pressure.

References:

[1] Ali A. Data-driven based machine learning models for predicting the deliverability of underground natural gas storage in salt caverns. Energy 2021;229:120648. https://doi.org/10.1016/j.energy.2021.120648.

[2] Berest P., Louvet F. (2020) Aspects of the thermodynamic behavior of salt caverns used for gas storage, OGST 75, 57.

[3] Evans J., Shaw T. (2021) Storage of hydrogen in solution mined salt caverns for long duration energy storage, in: Virtual Technical Conference, SMRI Spring 2021, April 2021.

SA-P08 MATEMATIC MODELING OF ADSORPTION ON ACTIVATED CARBON OF PETROLEUM GASES

Timur Chis[1*], Al Jaseem Ameer [2], Razvan Gaspar[2]

[1]Oil and Gas Engineering Faculty, Petroleum-Gas University

[2]Ph.D. School, Petroleum-Gas University

Abstract: *This paper presents the technologies for degasification of well gases with direct application to the treatment of well gases in the Black Sea.*
The C3+ fraction can be recovered from natural gas or can result from crude oil refining processes. The C3+ fraction recovered from well gases is practically free of unsaturated hydrocarbons (propylene and butylene) and results from one of the following extraction methods: turboexpander, absorption, compression and adsorption. The choice of process depends on the gas composition and the degree of recovery of ethane and C3+ fraction.
The C3+ fraction recovery facility at Midia is designed to process gases from the Central Platform located offshore the Black Sea. The LPG produced (mainly C3 and C4) will be stored in the tank farm. LPG can be used as household fuel, automotive fuel or feedstock for various petrochemical processes. The resulting lean gas will be compressed and shipped via the export pipeline.
In the study I conducted, I studied all types of installations used for the separation of rich gases, the technology for recovering lean gases through turboexpansion (cryogenics) as well as the calculation of a natural gas treatment plant.
I also introduced a chapter related to the risk assessment based on the event tree in the operation of these installations, which are particularly useful in the oil industry.
Key words: well gas, lean gas, degassing,

Introduction: The C3+ fraction can be recovered from natural gas or can result from crude oil refining processes. The C3+ fraction recovered from well gases is practically free of unsaturated hydrocarbons (propylene and butylene) and results from one of the following extraction methods: turboexpander, absorption, compression and adsorption. The choice of process depends on the gas composition and the degree of recovery of ethane and C3+ fraction [1].

Experimental and/or Modelling: The Midia C3+ recovery facility is designed to process gases from the Central Platform located offshore the Black Sea. The LPG produced (mainly C3 and C4) will be stored in the tank farm. LPG can be used as a household fuel, automotive fuel or feedstock for various petrochemical processes. The resulting lean gas will be compressed and shipped via the main export pipeline [2].

In the area of the facilities, leaks of liquid hydrocarbons and other compounds may occur, as well as emissions of vapors and gases from their handling, which can lead to pollution, fires or explosions.

LPG is volatile and flammable and must be stored and handled in special equipment. The risk due to LPG leaks can be analyzed by several methods. Risk

* Corresponding author: timur.chis@gmail.com

assessment involves analyzing the probabilities of the various consequences that have been identified during a safety study. To determine the frequency of accidents and their consequences, territorial information is necessary, such as the accident rate, meteorological conditions, environmental conditions, population risk.

After carrying out the risk analysis, technical and organizational measures will be required to eliminate or minimize the hazards in the facility.

Results and discussions: In this paper, the technological flow of the C3+ fraction recovery plant from well gases will be described. The risk factors and possible accident scenarios in this process will be identified. The methods for analyzing the risk generated by accidental LPG leaks will be briefly presented, with an emphasis on event tree analysis.

The risks in an LPG storage facility will be analyzed and measures to combat industrial risk will be proposed.

Finally, technical and occupational safety and toxicity standards in the C3+ fraction recovery plant from well gases will be presented.

Conclusion: I analyzed the gas chromatograms of the products resulting from adsorption on activated carbon, the purpose being to determine the amount of adsorbed product.

It is observed that the C4 fraction is absorbed best, for which the numerical model I made also gave the best results.

Activated carbon behaves very well at high pressures, the models made in Matchad giving quite good results.

The work is very well documented and with many applications being useful in the study of the separation of C3 + fractions.

References:

[1] Taylor, R. R., **Liquefied Petroleum Gas**, Kirk-Othmer Encyclopedia of Chemical Technology, Fifth Edition, John Wiley & Sons, Inc., 2007.

[2] American Institute of Chemical Engineers, **Guidelines for Chemical Process Quantitative Risk Analysis**, John Wiley & Sons, Inc., Second Edition, New York, 2000.

SA-P09 A NUMERICAL MODEL OF THE VOLATILE COMPOUNDS EMISSION TO OIL AND GASOLINE STORAGE

Iolanda Popa[1], Florina Casariu[1], Vasile Lavric[1], Timur Chis[2*],Sorin Steflea[3]

[1]Ph.D. School, National Science and Technology Politehnica University

[2]Oil and Gas Engineering Faculty, Petroleum-Gas University

[3]Ph.D. School, Petroleum-Gas University

Abstract: *This paper presents the method of calculating the losses of petroleum products during storage and transportation for different products generally handled in an oil terminal. An important element in determining the losses is also the environmental conditions in the location area (wind, sun, seismicity, etc.).There are several methods for determining the emissions of tanks with fixed or removable lids, the easiest being their determination by calculating the vapor balance. The basic model used in this study is a calculation model developed according to API standards, from which a proprietary methodology was developed and presented for estimating losses during the transport of various products. The study took into account both environmental factors (wind, temperature, tank paint color) and basic properties of the products such as density. The mathematical models that best correlated the data proved to be polynomial equations of degree 2 to degree 5. The simulations performed are among the first performed in this field, the determination of parameters with major influence being of major interest both for finding solutions to reduce losses on the service flow but also being opportune to develop mathematical models that correlate several parameters to facilitate the evaluation of these fugitive emissions.*

Key words: oil and product storage, volatile compounds emission, emission modelling,

Introduction: Emission sources and their contribution vary depending on the type of storage tank and occur as a result of evaporation of products during storage and as a result of changes in the liquid level.

Thus, in the case of tanks with a fixed lid, emissions are the result of evaporation losses during storage (also called breathing losses or static storage losses) and evaporation losses during filling and emptying operations (called working losses). Storage losses consist of the escape of vapors from a tank by the expansion and contraction of the vapor space as a result of temperature and pressure variations. This loss occurs without any change in the liquid level in the tank. The combined loss during filling and emptying is called working loss. As the liquid level rises, when the tank is filled, the pressure inside the tank exceeds the discharge pressure and the vapors are evacuated from the tank. Evaporative losses during emptying occur when the liquid level drops and the pressure also drops, so air enters the tank and the space allocated to the vapors expands and becomes saturated with air.

In the case of tanks with a fixed or movable cover, losses of petroleum products (emissions) vary depending on the capacity of the tank, the vapor pressure of the stored liquid and its rate of use. An important element in determining losses is also the environmental conditions in the location area (wind, sun, seismicity, etc.).

* Corresponding author: timur.chis@gmail.com

There are several methods for determining emissions from fixed or removable lid tanks, the easiest being to determine them by calculating the vapor balance.

Experimental and/or Modelling: The following presents the influence of various environmental factors and product quality on fugitive emissions. Among the environmental factors considered, we mention the tank temperature, wind speed, deterioration of the tank paint color.

The physicochemical parameters of the products considered were: density, REID vapor pressure [1].The parameter variation was considered to be between 55-90 kPa, which covers the entire range of values for the product specification in summer and winter conditions. If the operating losses remain constant with increasing vapor pressure, the storage losses increase with its increase.

Results and discussions :

Vapor pressure	Crude oil loss percentage (estimated) Kg of crude oil lost/tonne of product handled (maximum)	Equation
Vapour pressure, kPa	0,0014	$y = -0,0012x^4 + 0,3421x^3 - 35,967x^2 + 1682,8x - 27787$
Density, kg/m^3	0,0015	$y = -0,0012x^4 + 0,3421x^3 - 35,967x^2 + 1682,8x - 27787$
Wind , m/s	0,0055	$y = -0,0012x^4 + 0,3421x^3 - 35,967x^2 + 1682,8x - 27787$
Temperature ºC	0,0039	$y = 0,0172x^3 + 1,2868x^2 + 11,72x + 2009,5$
Mantle color condition	0,043	$y = 0,0172x^3 + 1,2868x^2 + 11,72x + 2009,5$

Conclusion: The simulations performed are among the first performed in this field, the determination of parameters with major influence being of major interest both for finding solutions to reduce losses in the service provision flow but also being opportune to develop mathematical models that correlate several parameters to facilitate the evaluation of these fugitive emissions.

References:

[1] *VOC Emission from Volatile Organic Liquid, Storage Tanks*, Background Information for Promulgated Standards, US Environmental Protection Agency, 1987,

SA-P10 STATISTICAL METHODS FOR EVALUATING THE QUALITY OF FINISHED OIL PRODUCTS

Iolanda Popa[1], Florina Casariu[1], Vasile Lavric[1], Timur Chis[2*],Sorin Steflea[3]

[1]Ph.D. School, National Science and Technology Politehnica University

[2]Oil and Gas Engineering Faculty, Petroleum-Gas University

[3]Ph.D. School, Petroleum-Gas University

Abstract: *Quality assurance by static methods is the stage that uses "statistical quality control sheets". In more and more companies, these methods are beginning to be applied, with an emphasis on the technological flow. The application of statistical sampling control methods has allowed the reduction of production costs. Statistical quality control is a sampling control method, in which the extracted sample (n) is controlled in its entirety, the results obtained allowing conclusions on the entire manufacturing process or on the finished products (N).In this regard, various statistical tools are used such as: data collection sheets, histograms, Pareto diagram, correction diagram, cause-effect diagram, dispersion diagram, control sheets. Advantages of applying statistical control methods: use of a small number of personnel, short decision-making time, operative establishment of adjustment and correction measures, ensuring the achievement and maintenance of process stability, reducing damage suffered by products, ensuring the delivery of product batches with specimens presenting defects within the limits jointly accepted by the supplier and beneficiary.*
Key words: product analysis, statistic modelling, quality,

Introduction: This study is based on the quality control of the main white petroleum products. The quality control was carried out in a RENAR accredited laboratory.

Thus, the following quality parameters were analyzed:

- for gasoline – density, sulfur
- for oil – density, current gums
- for diesel – density, sulfur, lubrication point.

These parameters were analyzed because:

- density - provides information on the composition. Knowing the density provides information on fuel consumption and their calorific value. Calorific value - It is given by the amount of heat that is released upon complete combustion of a kg of fuel or cubic meters of gaseous fuel and is expressed in kcal or kj. The value of the calorific value depends on the chemical composition of the fuel and in particular on its H and C molecules.
- sulfur - quality control regarding the minimum sulfur content, in the case of fuels, is an essential requirement according to the emission regulation and indicates the tendency of combustion products to corrode.

* Corresponding author: timur.chis@gmail.com

- actual rubbers - the rubber content gives indications on the danger of solid deposits formation due to fuel degradation, with implications on the proper functioning of the engine.
- lubrication point - the fuel must provide the necessary lubrication capacity for an efficient engine lubrication system [1].

Experimental and/or Modelling: Quality assurance through statistical methods is the stage that uses "statistical quality control sheets". In more and more companies, these methods are beginning to be applied, focusing on the technological flow. The application of statistical control methods through sampling has allowed the reduction of production costs.

Investing in quality is one of the best investments that a company can make today; it is a privileged means of lowering the return price, increasing the added value, retaining customers and winning new market segments - the goal is to make the company increasingly competitive. For the analysis and evaluation of quality, in parallel with the existence of classical methods, new methods have emerged (affinity diagrams, tree diagrams, relationship diagrams) that allow the identification of the causes of defects, the prioritization of actions for improvement.

Results and discussions : Quality analysis aims to:

- knowledge of the methods and means of achieving quality and the option for an optimal solution in a given case.
- comparison of the quality level of a product at different manufacturing intervals or comparison with the similar product of other companies [16].

Conclusion: In parallel with the rapid technological and socio-cultural changes, the methods of ensuring the quality of products and services have also evolved. Four stages can be considered in the evolution of the methods of quality assurance:

- Quality assurance through control
- Quality assurance through statistical methods
- Quality assurance through staff motivation
- Integrative concepts of quality assurance.

References

[1] A.Raznat, *Lubricity Improvement of the Ultra-low Sulfur Diesel Fuel with the Biodiesel*, Energy Procedia 75, p.111-117, 2015,

SA-P11 STRUCTURE EQUATIONS OF TERMAL ROCKS AI MODELS

Ioana Purghel[1], Maria Stoicescu[2*], Claudiu Dolete[1]

[1]Ph.D. School, Petroleum-Gas University

[1]Geological and Oil Engineering, Petroleum-Gas University

Abstract: *Geothermal energy, sourced from the Earth's internal heat, is a key renewable resource. This study focuses on the geothermal potential of the Ploiești subsoil, where a consistent thermal gradient is observed. At a depth of 100 meters, temperatures are constant year-round, ranging from 13.2°C to 13.8°C depending on the rock composition. The reliability of this low-enthalpy geothermal field makes it suitable for industrial use. To explore this potential, we have developed a numerical model to simulate the thermal behavior of the area's rock formations.*
Key words: Thermal rocks, ANNs model, Environment Simulation

Introduction: Geothermal energy is unique among renewables because it arises from the Earth's own internal heat, not the sun. This heat comes from two distinct sources. The first is primordial heat, a 4.5-billion-year-old legacy from the planet's formation, with core temperatures still over 5000∘C [1]. The second is radiogenic heat, which is constantly produced by the radioactive decay of elements like uranium, thorium, and potassium in the crust and mantle [2]. This radiogenic process is responsible for about half of the Earth's surface heat flow [3].These two sources combine to produce a continuous heat output of about 44.2 TW [34]. This constant, internal heat production makes geothermal an exceptionally reliable and sustainable resource on a geological scale, unlike finite fossil fuels or intermittent renewables like solar and wind [3].

Experimental and/or Modelling: In the UPG Ploiești area the average water temperature is 8.92 ℃, the average basement temperature is 16.8 ℃, the average loss of basement temperature (due to water injection) is 6.33 ℃ and the average loss of water temperature (due to use in the heat pump) is 4.11 ℃. At a flow rate of 3 mc/h the variation of the extracted power (kW) as a function of the temperature difference is shown in figure 1.

Results and discussions : Also, for the first time in the literature, we simulated the value of geothermal energy extracted by a well and then used the data to generate, train and evaluate four different Artificial Intelligence (AI) models.

This simulation started from the creation of a numerical model that would provide us with data on the variation of geothermal power with respect to the depth of the well and the type of rock through which the water flows

I generated a dataset with 500 records.

* Corresponding author: stoicescu.maria@yahoo.com

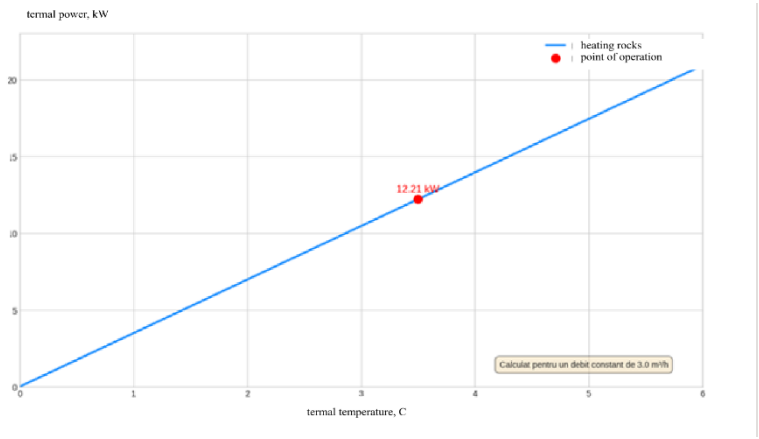


Fig. 1 Variation of thermal energy extracted from a water well as a function of the temperature difference given off

The model equations are:

Linear Regression

Power_kW = -1.8696 + (0.0748 * Depth) + (0.2419 * Flow) – (1.9598 * RockType_Dry Clay) + (1.0953 * RockType_Limestone) + (3.0403 * RockType_Granite) + (2.0691 * RockType_Sandstone) (5.5)

Ridge Regression

Power_kW = -1.8163 + (0.0748 * Depth) + (0.2418 * Flow) – (1.9844 * Dry_Clay_RockType) + (1.0332 * Limestone_RockType) + (2.9529 * Granite_RockType) + (1.9943 * Sandstone_RockType) (5.6)

Conclusion: Some older studies mention that the (shallow) groundwater in the southern and southeastern areas of the municipality may be contaminated with petroleum products. This is an important factor to consider and requires a water quality analysis before designing an open geothermal system.

References:

[1] Bini, R., Manciana, E., - Organic Rankine Cycle Turbogenerators for Combined Heat and Power Production from Biomass. In: Proceedings of the 3rd Munich Discussion Meeting 1996, ZAE Bayern (ed.), Munich, Germany, 1996.

[2] Claesson, J. And P. Eskilson – Conductive Heat Extraction to a Deep Borehole, Thermal Analysis and Dimensioning Rules. Energy 13/6, 2024

[3] Feidt, M. - Thermodynamique et Optimisation Energetique de Systemes et Procedes, Technique et Documentation (Lavoisier), Paris, 2024

SA-P12 NUMERICAL MODELS TO OIL WATER EMULSION

Aurelian Șisinea[1], Florin Bogdan[1], Mihai Albulescu[2*],

[1]Ph.D. School, Petroleum-Gas University

[2]Oil and Gas Engineering Faculty, Petroleum-Gas University

Abstract: *The growing thirst for energy from hydrocarbons leads to the use of all possibilities for the extraction, transport and storage of crude oil from Romanian deposits.That is why viscous crude oils are extracted to be processed in a mixture with freezable crude oils, in order to obtain refining products with a low processing cost.Viscous crude oils are also useful in the production of bitumen and that is precisely why their extraction is necessary. This paper analyzes the possibilities of transporting viscous crude oils in emulsion (both from the point of view of the stability of the emulsions and especially from the point of view of the rheological characteristics of transport). Even if emulsions can create problems in pipeline transport (by separating and decanting the water present in the emulsion), currently it is possible to create installations that do not lead to the deposition of water in the roughness of the pipes and therefore this transport is profitable and useful.*
Key words: oil emulsion, pipeline, viscous,

Introduction: The United States Department of Energy (USA) forecasts an increase in the amount of crude oil in the next 20 years from 60 million barrels per day to 84 million barrels per day.

In this context, the oil industry is currently looking for new crude oil deposits and especially the exploitation of unconventional deposits (crude oil stored in clays or sands, crude oil from oil shale, etc.).

Solutions are also being sought for the extraction, transport and processing of heavy crude oil (asphaltic and bituminous), which in Romania alone account for over 50% of the total extracted crude oil.

In Canada, about 700,000 barrels of crude oil are extracted per day from oil sands and oil shale.

The decline in medium and light oil reserves and the drop in crude oil prices make the exploitation of heavy (asphaltic) deposits unprofitable by classical methods (solvent extraction, polymer extraction, underground combustion).

Conventional reserves of heavy crude oil are estimated at 6 billion barrels, with Canada, Romania and Venezuela being the main countries that exploit and transport such crude oil through pipelines.

That is why over the years various methods of treating this type of crude oil have been tried for transport.

Experimental and/or Modelling: A first option was the heated transport of heavy crude oils, which was difficult to achieve both due to high costs and especially due to technological conditions (separation of water from crude oil after heating, sudden cooling in case of damage, etc.).

* Corresponding author: malbulescu@upg-ploiesti.ro

Another method often used was mixing with diluents (light crude oils, naphtha, etc.).

This process is also unusable due to the deterioration of the quality of the mixed crude oils.

The best solution is to deliver emulsified crude oils because:

a. It does not require heating along the route,

b. Reservoir water can be used as an emulsifier (to be transported to a treatment plant),

c. Energy consumption is greatly reduced, even by 40%,

d. Water-in-crude emulsions can be used for low consumption, but also crude oil-in-water emulsions (only in an 80-20 ratio),

e. It has been observed that asphaltenes have the greatest influence on viscosity, compared to other types of crude oils.

Even though emulsions can create problems in pipeline transport (by separating and settling the water present in the emulsion), currently it is possible to create installations that do not lead to the deposition of water in the roughness of the pipes and therefore this transport is cost-effective and useful.

During this period of time, research is focused on the concentric transport of crude oil mixed with reservoir water.

Conclusion: From the laboratory analyses performed and from the study of the specialized literature, the following conclusions were drawn:

- emulsification leads to a decrease in viscosity only when a mixture ratio of 80-20 and 40-60 water-crude oil is used,

- the data from the specialized literature are confirmed, namely the transport of emulsified crude oil can only be done in an emulsion of the crude oil-in-water type,

- it is also observed that distilled water ensures better emulsification compared to reservoir water,

- it is interesting that at the proportion of 40-60 water in crude oil, the viscosity increases suddenly, beyond the viscosity limits even of the compounds used, this phenomenon being explained in the specialized literature by the phenomenon of emulsion inversion,

References:

[1]. Dake, L.P., Abarasi Hart, *A review of technologies for transporting heavy crude oil and bitumen via pipelines,* J Petrol Explor Prod Technol, DOI 10.1007/s13202-013-0086-6,

SA-P13 ANALYSIS OF VOLATILE COMPOUNDS EMISION TO OIL STORAGES

Maria Stoicescu[1*], Sorin Steflea[2], Iolanda Popa[3], Vasile Lavric[4]

[1]Oil and Gas Engineering Faculty, Petroleum-Gas University

[2]Ph.D. School, Petroleum-Gas University

[3]Ph.D. School, Politehnica University

[4]Național Science and Technology Politehnica University

Abstract: *In the case of volatile organic compounds that may occur following the This paper presents the method of calculating the losses of petroleum products during storage and transportation for different products generally handled in an oil terminal. An important element in determining the losses is also the environmental conditions in the location area (wind, sun, seismicity, etc.).There are several methods for determining the emissions of tanks with fixed or removable lids, the easiest being their determination by calculating the vapor balance. The basic model used in this study is a calculation model developed according to API standards, from which a proprietary methodology was developed and presented for estimating losses during the transport of various products. The study took into account both environmental factors (wind, temperature, tank paint color) and basic properties of the products such as density. The mathematical models that best correlated the data proved to be polynomial equations of degree 2 to degree 5. The simulations performed are among the first performed in this field, the determination of parameters with major influence being of major interest both for finding solutions to reduce losses on the service flow but also being opportune to develop mathematical models that correlate several parameters to facilitate the evaluation of these fugitive emissions.*

Key words: volatile compounds emission, emission modelling,

Introduction: The technological losses that occur when storing petroleum products and crude oil in the storage tank are due to the phenomenon of expansion of the air-vapor mixture of petroleum product (daytime) and thermal contraction of the air-vapor mixture of petroleum product (nighttime). Thus, the expansion of the vapor-air mixture in the vapor space of the tank leads to an increase in the vapor pressure up to the maximum venting pressure value (which is set on the safety valve or the breathing valve. When this pressure is reached, the valve opens and allows the petroleum product vapors to dissipate into the atmosphere.

Thermal cooling of the ambient environment produces the opposite phenomenon, namely the contraction of the vapor-air mixture and implicitly a decrease in pressure. When the pressure in the free liquid space in the tank drops below the minimum venting pressure value (which is set on the safety valve or the breathing

* Corresponding author: maria.stoicescu@yahoo.com

valve), the air from the atmosphere enters the vapor space of the tank and then becomes partially saturated with vapors from the stored product.

Experimental and/or Modelling: Also, the daily heating-cooling cycle due to solar radiation or changes in ambient temperature leads to changes in the temperature of the tank cover and jacket. This change causes a heat exchange between the air-vapor mixture in the tank vapor space and the tank jacket, causing a convection movement of the air-vapor mixture in the tank vapor space. In addition, evaporation of the upper layer of the liquid petroleum product in the tank occurs at the surface of the liquid, as the stored product tries to achieve equilibrium conditions with the air-vapor mixture in the tank vapor space. They occur during the daily heating-cooling cycle. At the same time, the phenomenon of vapor diffusion also occurs, from the surface of the liquid stored in the tank to the area below the "vent". Convection and diffusion of vapors leads to a change in their saturation degree [1].

Results and discussions : This paper presents the method of calculating losses of petroleum products during storage and transportation for different products generally handled in an oil terminal. An important element in determining losses is also the environmental conditions in the location area (wind, sun, seismicity, etc.).

Conclusion: The simulations performed are among the first performed in this field, the determination of parameters with major influence being of major interest both for finding solutions to reduce losses in the service provision flow but also being opportune to develop mathematical models that correlate several parameters to facilitate the evaluation of these fugitive emissions.

References:

[1] A J Venn, M Cooper, M Antoniak, C Laughlin, J Britton, S A Lewis, "*Effects of volatile organic compounds, damp, and other environmental exposures in the home on wheezing illness in children*", Thorax 2003;58:955–960, 2003,

SA-P14 APPLICATION OF THE GAMMA FUNCTION IN OIL RESERVOIRES POLYMER INJECTION MODELING

Mihai Virtopeanu[1], Maria Stoicescu[2*],

[1]Ph.D. School, Petroleum-Gas University

[2]Geological and Oil Engineering, Petroleum-Gas University

Abstract: *In this paper* we analysis *the applicability of the Gamma function in modeling the behavior of polymers injected into reservoirs was studied, having as data for validation the results of the implementation of this process on reservoir X. This reservoir, with well-documented lithological and petrophysical characteristics, provides an adequate framework for testing the validity of theoretical models and for their extrapolation into real operational scenarios. By integrating the Gamma function within advanced modeling, the aim is to obtain a robust analytical tool, capable of contributing to improving technical decisions regarding the selection of operational parameters, the evaluation of recovery efficiency and the prognosis of reservoir performance under polymer injection regime.*

Key words: Gamma function, Oil reservoires, Polimer injection

Introduction: Enhanced Oil Recovery (EOR) is an essential component in optimizing the recovery factor from mature reservoirs, contributing to extending the economic life of oil fields. In the context of natural decline in production and increasing economic and environmental pressure, For the design, control and optimization of this process, it is essential to use mathematical models capable of accurately describing the behavior of polymers in the porous medium.

Experimental and/or Modelling: The polymer transport process in a fluid-saturated porous medium is governed by advection (movement caused by fluid flow), dispersion (mechanical diffusion due to microscopic heterogeneities of the medium) and, in some cases, adsorption or degradation reactions [1].

For a homogeneous, isotropic medium without chemical reactions, the transport equation describing the propagation of polymer concentration is [2]:

$$\frac{\partial C}{\partial \mathrm{t}} + \mathrm{v}\frac{\partial C}{\partial \mathrm{x}} = D\frac{\partial^2 C}{\partial x^2} \qquad (1)$$

where:

C(x,t), represents the polymer concentration as a function of space (x) and time (t),

v is the fluid flow velocity,

D is the longitudinal dispersion coefficient.

Results and discussions : The integration of the gamma model into the analysis of reservoir X led to:

* Corresponding author: stoicescu.maria@yahoo.com

- a better understanding of the behavior of the polymer in heterogeneous porous media,

- improved decisions regarding the placement of observation wells and injection parameters,

- the possibility of building predictive scenarios in order to extend the injection to other sectors of the reservoir.

Here is the plot of the polymer concentration in the reservoir *C(x)* vs. the distance (*x*) of penetration of the polymer solution into the reservoir, which compares different shapes of the Gamma distribution as a function of the parameters *k* and θ, including the calibrated case for reservoir X (*k*=1.8; θ=60).

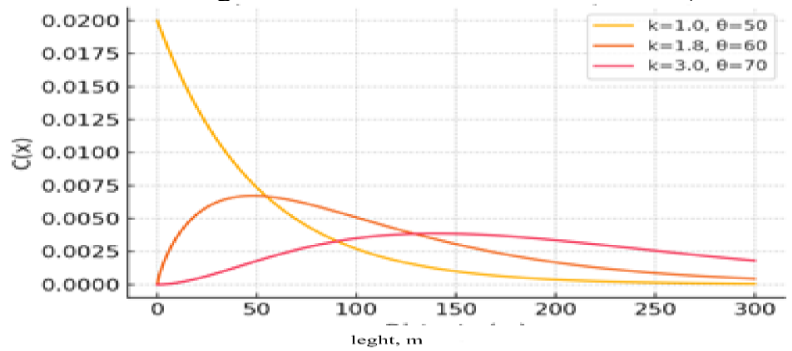


Fig.1. Gamma distribution

- The yellow curve (k=1; θ=50) has an exponential shape, typical of simple transport, without significant dispersion.

- The orange curve (k=1.8; θ=60) shows a clear peak and an extended tail – realistic behavior observed in polymer injection at reservoir X.

- The red curve (k=3; θ=70) is more symmetrical, with a more uniform spread – characteristic of more homogeneous media.

This graph helps to compare different injection scenarios and can be integrated into the paper to support the choice of the gamma model.

Conclusion: The paper demonstrated the applicability of the Gamma function in modeling the polymer injection process in a porous medium representative of a mature oil reservoir.

References:

[1] Lake, L. W. (1989). *Enhanced Oil Recovery*. Prentice Hall. Shook, G. M., & Lake, L. W. (1995). *Polynomial and power-law solutions to the convection–dispersion equation*. SPE Journal, 10(2), 85–93.

[2] Bear, J. (1972). *Dynamics of Fluids in Porous Media*. Dover Publications.

SA-P15 CHARACTERISATION AND ANALYTICAL IDENTIFICATION OF POLYAROMATICS FROM DIESEL FUEL

Bianca Simedrea[1*], Nicoleta-Oana Demostene[1], Iuliana Deleanu[1], Oana Parvulescu[1], Olga Sapunaru[2], Tănase Dobre[1]

[1]National University of Science and Technology POLITEHNICA Bucharest, 1-7 Gheorghe Polizu Str., 011061 Bucharest, ROMANIA, [2]Universitatea Ovidius Constanta, 124 Mamaia Boulevard, 900527 Constanța, ROMANIA

Astract: *In this study, different diesel fuel samples were analyzed to see the effects of polyaromatics on engine combustion compared to European standards. Different diesel fuel samples from HPM and HDV plants were evaluated over 60 days to observe the variation of the aromatics content in diesel fuel over a longer period of time. The monitoring of polyaromatics was performed using the HPLC chromatographic method and plant operating parameters.*

Key words: diesel, polyaromatics, chromatography, engine, standards, aromatics, exhaust emissions, plants

Introduction: Polycyclic aromatic hydrocarbons (PAHs) are persistent organic compounds composed of 2 to 7 benzene rings, commonly found in the environment as microparticules (PM10), primarily resulting from fossil fuel combustion. PAHs originate from pyrogenic, petrogenic and biological processes, with pyrogenic PAHs forming under high temperatures and low oxygen conditions, and petrogenic PAHs arising from crude oil and related activities. PAHs particulate phase have been found in the atmospheres of urban, industrial and rural areas and even in indoor air. Moreover, they are one of the air pollutants of greatest concern to human health due to their carcinogenic, mutagenic, genotoxic and immunosuppressive effects [1,2]. In addition, some PAHs and their derivatives are considered endocrine disruptors. As such, they are considered priority pollutants by the United States Environmental Protection Agency (EPA) and the International Agency for Research on Cancer. Due to the important environmental effects of PAHs, extensive studies have been conducted in recent years on the concentrations of PAHs in the particulate and gas phases [1,3,4].

Experimental: Different samples of Euro 5 diesel fuel, from different batches prepared for sale, were tested to see the amount of aromatics using HPLC chromatography. The analysis was conducted with an Agilent 1260 HPLC system employing 100% heptanes as the mobile phase, a refractive index detector, and a column thermostat set at 30°C. Samples were prepared by precise weighing and dilution in n-heptane, followed by chromatographic comparision against regulatory standards. They were compared with each other and with the norms imposed by the legislation to see if the batches meet the imposed conditions.

* Corresponding author: Email address:

The PAHs analysis was integrated into the monitoring of HPM and HDV hydrogenation units. These units process different blends of gas oils and kerosene under catalytic hydrogenation conditions to reduce sulfur, nitrogen, oxygen compounds, aromatics and olefins. Key process variables such as: feed density, flow rates, temperature and sulfur content were correlated with output parameters including product sulfur concentration, density and PAHs levels.

Results and disscusions: This study investigates the variation of polyaromatic hydrocarbon (PAH) content in diesel fuel in relation to reactor operating parameters. Data analysis reveats that polyaromatic concentrations descrease with increasing density at both the inlet and outlet of the reactor, while a reduction in sulfur levels at the outlet coresponds with an increase in PAH content. Despite these fluctuations the Euro 5 diesel samples from the test batches contain polyaromatics values that fall within the norms imposed by the government. The value differs depending on the operating parameters of the installations, as well as the installation from which the samples come. A lower content of polyaromatics and sulfur is observed in the HDV installation, compared to the HPM installation. HC, PM, NOx emissions increase with the addition of mono-, di- and triaromatics. PM emissions are the ones that increase more than HC AND NOx.

Conclusions: The differences in the traffic fuels have been shown to affect exhaust emissions and their toxicity. Especially, the aromatic content of diesel fuel is an important factor considering the emissions, notably particulate matter (PM) concentrations. The ultra-fine particles (UFP, particles with a diameter of <100 nm) are important components of engine emissions and connected to various health effects, such as pulmonary and systematic inflammation, and cardiovascular disorders. Studying the toxicity of the UFPs and how different fuel options can be used for mitigating the emissions and toxicity is crucial.

References:

[1] Glugorijevic R., Jevtic J., Borak D., The influence of fuel aromatics on diesel exhaust emission *Journal of KONES Powertrain and Transport*, 14 (2), 161-170, 2007.

[2] Pěnčíková K., Ciganek M., Neča J., Illés P., Dvořák **Z.**, Vondráček J., Machala M., Modulation of endocrine nuclear receptor activities by polyaromatic compounds present in fractionated extracts of diesel exhaust particles, *Sci. of The Total Envir.,* 677, 626 – 636, 2019

[3] Lin Y. C., Lee W. J., Chen C. B., Characterization of Polycyclic Aromatic Hydrocarbons from the Diesel Engine by Adding Light Cycle Oil to Premium Diesel Fuel, *Journal of the Air & Waste Manag. Assoc.*, 56(6), 752–758, 2006.

[4] Salonikidou E. D., Kowalska K., Giannakoudakis D. A., Margello A., Nanaki E., Kiartzis S., Barczak M., Borowski P., Triantafyllidis K. S. , Merging experimental and theoretical approaches towards understanding real diesel fuel desulfurization by nanoporous carbons, *Chem. Eng. Journal,* 502, 157858, 2024.

SA-P16 THERMODYNAMIC CONSIDERATIONS REGARDING DIESEL HYDRODESULFURIZATION

Laura Elisabeta Petras[1,2*], Claudia Muntean[3] , Tănase Dobre[1]

[1]Chemical and Biochemical Engineering Department, University POLITEHNICA of Bucharest, 1-7 GheorghePolizu Str., 011061 Bucharest

[2]Petromidia Refinery, NavodariBld 214, Navodari 905700

[3]Chemistry and Chemical Engineering Department, Ovidius University 124 MamaiaBld 900527

Abstract: This paper presents a thermodynamic analysis of the diesel hydrodesulfurization (HDS) process, focusing on the influence of operational conditions such as temperature, pressure, hydrogen-to-oil ratio, and catalyst type on sulfur removal efficiency. The study highlights the equilibrium aspects governing hydrogenation and desulfurization reactions, emphasizing the competing routes of direct desulfurization (DDS) and hydrogenation (HYD). Comparative assessment between catalytic and non-hydrogenative desulfurization methods (adsorptive and extractive) is discussed, underlining the industrial relevance of HDS due to its superior sulfur conversion and process stability. Thermodynamic evaluations confirm that higher temperatures and hydrogen partial pressures shift the equilibrium toward hydrogen sulfide formation, favoring complete sulfur removal.

Key words: Diesel hydrodesulfurization, thermodynamic analysis, Co–Mo/Al_2O_3 catalyst, Ni–Mo/Al_2O_3 catalyst, hydrogenation, sulfur removal, process optimization.

Introduction: The hydrodesulfurization (HDS) of diesel fuels is a crucial catalytic process for producing ultra-low sulfur diesel (ULSD) compliant with environmental regulations. Sulfur compounds such as thiophenes and benzothiophenes are converted into hydrogen sulfide via hydrogenation reactions in the presence of sulfided Co–Mo or Ni–Mo catalysts. Understanding the thermodynamic behavior of these reactions is essential for optimizing energy consumption, catalyst life, and overall refinery performance.

Experimental and/or Modelling: Thermodynamic analysis was conducted considering equilibrium constants and Gibbs free energy changes for key reactions involved in HDS. Operating parameters—temperature (300–400 °C), pressure (30–130 bar), and hydrogen partial pressure—were varied to determine their effect on equilibrium composition. Data from industrial HDS units were compared with simulation results obtained using ASPEN Plus thermodynamic modules. The study also evaluated the feasibility of alternative desulfurization methods such as liquid–liquid extraction and adsorption for comparison purposes.

Results and Discussions: Results indicated that the equilibrium conversion of organosulfur compounds increases with both temperature and hydrogen partial pressure, confirming the endothermic nature of the desulfurization reactions. Ni–

* Corresponding author: laurapetras@yahoo.com

Mo catalysts, which promote hydrogenation, demonstrated higher sulfur removal efficiency for complex aromatic species such as dibenzothiophenes, while Co–Mo catalysts favored direct desulfurization pathways. Non-hydrogenative methods such as adsorption on modified polymers or zeolites showed limited efficiency and poor regeneration capacity. Overall, thermodynamic evaluation supports HDS as the most viable large-scale process due to its high sulfur conversion, catalyst stability, and integration with hydrogen management systems.

Conclusions: Thermodynamic analysis confirms that hydrodesulfurization remains the most effective technology for achieving ultra-low sulfur diesel production. The process benefits from high equilibrium conversion at elevated temperatures and pressures, provided that hydrogen supply and catalyst properties are optimized. While alternative desulfurization techniques offer potential niche applications, catalytic HDS remains unmatched in industrial efficiency, selectivity, and environmental compliance.

References:

[1] Jimenez F., Nunez M., Kafarov V. (2005). *Study and modeling of simultaneous hydrodesulfurization, hydrodenitrogenation and hydrodearomatization on vacuum oil hydrotreatment.* In: European Symposium on Computer-Aided Processes, Elsevier Science.

[2] Babich I. V., Moulijn J. A. (2003). *Science and technology of novel processes for deep desulfurization of oil refinery streams: A review.* Fuel, 82, 607–631.

[3] Chowdhury R., Pedernera E., Reimert R. (2004). *Trickle-bed reactor model for desulfurization and dearomatization of diesel.* AIChE J., 48, 126–135.

[4] Saajanlehto M., Uusi-Kyyny P., Alopaeus V. (2014). *Hydrogen solubility in heavy oil systems: experiments and modeling.* Fuel, 137, 393–404.

[5] Baloochy B., Shokri S., Marvasar A. M. (2010). *Design and implementation of simulator for hydrotreating reactor in RTO development.* Int. J. Chemical Engineering and Applications, 1(4), 287–293.

[6] Novaes L. R., Resende N. S., Salim V. M., Secchi A. R. (2017). *Modeling, simulation and kinetic parameter estimation for diesel hydrotreating.* Fuel, 209, 184–193.

[7] Wang S., Liu Q., & Zhang Y. (2019). *AI-based predictive control for hydroprocessing units.* Chemical Engineering Research and Design, 148, 22–35.

[8] Mederos F. S., Ancheyta J. (2007). *Mathematical modeling and simulation of hydrotreating reactors: cocurrent versus countercurrent operations.* Applied Catalysis A: General, 332, 8–21.

[9] Murali C., Voolapalli R. K., Ravichander N., Gokak D. T., Choudary N. V. (2007). *Trickle-bed reactor model to simulate the performance of a commercial diesel hydrotreating unit.* Fuel, 86, 1176–1184.

[10] Dobre T., Petras L. E. (2024). *Industrial data-driven modeling of diesel HDS reactor performance.* Romanian Chemical Engineering Society Bulletin, 75(2), 115–129.

SA-P17 PROCESS SIMULATION OF CITRIC ACID BIOSYNTHESIS WITH SuperPro Designer®

Mihai Tone [1], Iuliana Mihaela Deleanu [1], Gabriela Isopencu [1*], Alexandra Mocanu [1,2*]

[1]NUST POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, Dept of Chemical and Biochemical Engineering, Polizu St 1-4, Bucharest, Romania

[2]National Institute for Research and Development in Microtechnologies (IMT Bucharest), 126A Erou Iancu Nicolae Street, 077190 Voluntari (Ilfov), Romania

Abstract: *The purpose of the paper is to present a simulation of the entire technological process of obtaining citric acid, carried out in SuperPro Designer v8.5. Based on the results obtained in the simulator, the calculation sheets for the entire procedure (mass, energy, economic aspects) were extracted to highlight the reliability of the process. The simulation result indicates a purity of >99.5% of the final product, with an estimated time of 9 days for fermentation process. The mass conversion ratio of molasses to citric acid is 51%, with a production of approx. 1365 kg of product per batch. Using the economic model of the embedded simulator, the investment value was determined at 69.3 million USD, with an annual profit of 11 million USD, assuming a payback period of 10 years.*

Key words: citric acid, process simulation, *Aspergillus niger*

Introduction: The first synthesis of citric acid by fermentative route was achieved by Carl Wehmer using *Penicillium* (known then as *Citromyces*) which accumulates citric acid in a culture medium initially rich in sugars and inorganic salts. Other fungi that have been studied for their potential to synthesize citric acid were *Aspergillus sp., Absidia sp., Acremonium sp., Botrytis sp., Eupenicillium sp., Mucor piriformis, Penicillium janthinellum, Penicillium restrictum, Talaromyces sp., Trichoderma viride, and Ustulina vulgaris* [1]. The production of citric acid is a well-known process, which involves three main stages: i) the fermentation phase which includes the preparation of the culture medium, preparation of the inoculum and the bioreaction itself; ii) the separation phase which involves on the one hand the separation of the microbial biomass from the broth, and on the other hand the separation of citric acid from the liquid medium, using different techniques (precipitation, solvent extraction, membrane filtration, etc.) and, iii) purification/concentration stage, which in turn could include several methods (acidification, ion exchange, adsorption, crystallization) followed by drying of the obtained crystals [2],[3].

Process simulation: To conceptually visualize a citric acid production plant incorporating the aforementioned steps, a simulation software is utilized to generate the process flow diagram. In this case, the simulation was conducted using

* Corresponding author: gabriela.isopencu@upb.ro
* Corresponding author: alexandra.mocanu@imt.ro

SuperPro Designer v8.5, a chemical process simulator specifically designed for large scale bioprocesses.

Results and discussions: The paper presents the simulation of a possible industrial process for the synthesis of citric acid by fermentative route, and certain aspects related to the optimization of its performance. Through the analysis thus presented, it can be concluded that the process is in continuous development, but the procedures for obtaining citric acid by biological routes remain still optimal. Figure 1 shows the simulation of the bioprocess section - fermentation stage of the citric acid production process, in batch operation, using *A. niger* as the producing strain, on molasses substrate.

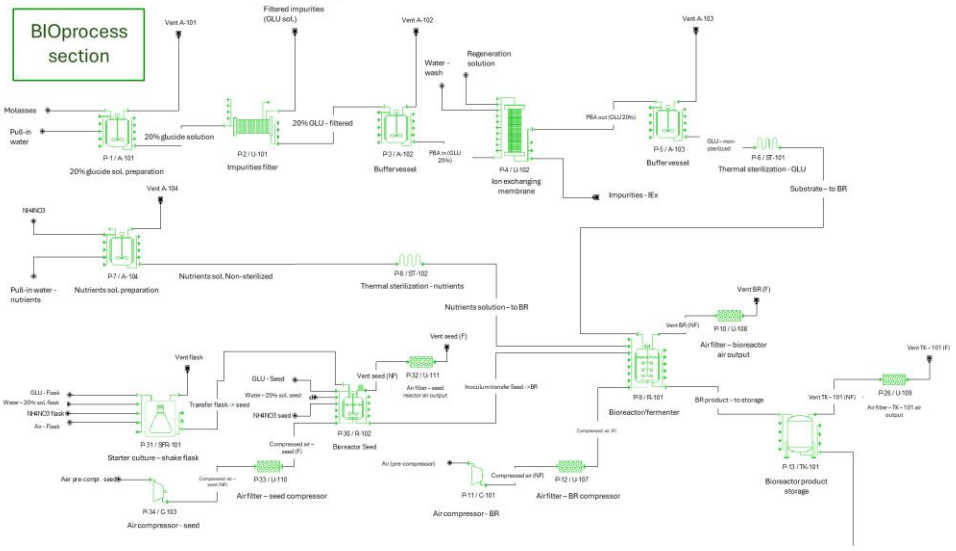


Fig. 1 Fermentation section in process simulation.

Conclusions: The results indicate that the analysis of biological syntheses can lead to the discovery of more environmentally sustainable processes, thus integrating the use of various wastes obtained from other production processes.

References:

[1] Papagianni M., *Advances in citric acid fermentation by Aspergillus niger: Biochemical aspects, membrane transport and modeling*, 2007. Biotechnology Advances 25/3, 244-263.doi: 10.1016/j.biotechadv.2007.01.002.

[2] Woinaroschy A. și Lavric V., „Kinetic models for citric acid production”. [Online]. Disponibil la: https://www.researchgate.net/publication/237051730

[3] Książek, E. Citric Acid: Properties, Microbial Production, and Applications in Industries. *Molecules* **2024**, *29*, 22. https://doi.org/10.3390/molecules29010022

SA-P18 MODELING THE THERMAL PROCESS IN CURING HIGH CONSISTENCY SILICON RUBBER

Raluca Isopescu and Paula Postelnicescu

National University of Science and Technology Politehnica Bucharest

Abstract: *The heat transfer during the curing of high consistency silicon rubber (HCR) with peroxide is studied using Matlab.*
Key words: HCR vulcanization, heat transfer modelling.

Introduction: Curing or vulcanization process is a fundamental step during the manufacturing of rubber articles. It plays an important role in achieving accurate and low tolerance shape and pre-designed physical and mechanical properties of the final product [1]. During vulcanization, the long chains of the elastomer chemically cross-link. In the curing process, the extent of reaction or degree of cure requirement represents ≥ 90% crosslinking for optimal performance and the typical temperature is between 170-200°C. The variation of temperature and degree of cure in a High Consistency Silicon Rubber (HCR) bar during compression molding were analyzed.

Modeling: The heat transfer with generation by chemical reaction is considered in the thickness of the bar as the geometry of the bar is simple and the length is much higher than the bar thickness.

Heat transfer equation:

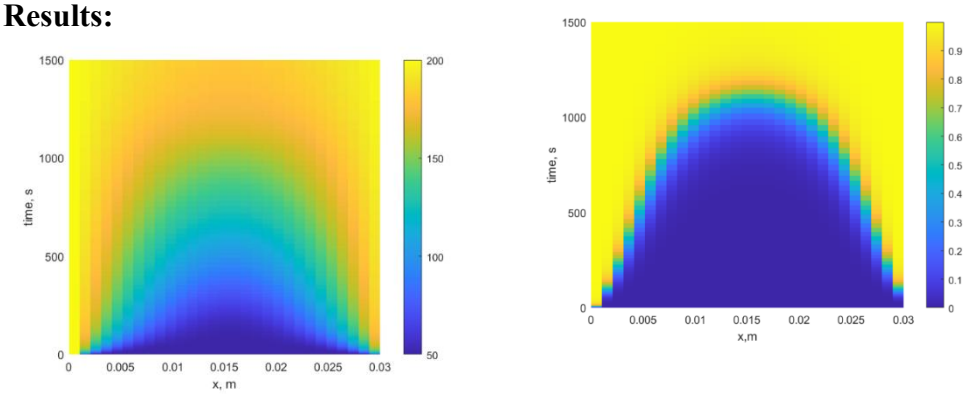
$$\frac{\partial T}{\partial \tau} = \frac{k}{\rho \cdot c_p} \cdot \frac{\partial^2 T}{\partial x^2} + f \tag{1}$$

The kinetic equation defines the variation of the degree of cure, y [2]:

$$\frac{dy}{d\tau} = \left(k_1 + k_2 \cdot y^m\right) \cdot \left(1 - y\right)^n \tag{2}$$

The model was solved in Matlab 2023 by defining the geometry of the bar and the materials properties. Eq (1) was discretized in the nodes of a mesh created in the thickness of the HCR bar and coupled with eq (2). The system was integrated using ode15s implemented in Matlab.

Results:



a **b**

Variation of temperature (a) and degree of cure (b) during the thermal process

References:

[1] Ghoreishy, M., H., R., A state of art review on the mathematical modeling and computer simulation of rubber vulcanization process, *Iran Polym J.*, 25(1), 2016, 89-109.

[2] Azvedo, M., Monks, A. M., Kerschbaumer, R., Schlogl, S. and Holzer, C., Peroxide-Based Crosslinking of Solid Silicone Rubber. Part I: Insights into the Influence of Dicumylperoxide Concentration on the Curing Kinetics and Thermodynamics Determined by a Rheological Approach, *Polymers,* 14(20), 2022, DOI: 10.3390/polym14204404

SA-P19 METHODS FOR THE REMOVAL OF IBUPROFEN FROM WATER

Florina Lungu (Ionita) [1*], Daniela Simina Ștefan[2*]

[1]. PhD student, Faculty of Chemical Engineering and Biotechnology National University of Science and Tehnology Politehnica,, str.Polizu 1-7 district, Romani

[2] Faculty of Chemical Engineering and Biotechnology National University of Science and Tehnology Politehnica, str.Polizu 1-7 district, Romania

Abstract: *Ibuprofen, one of the most widely used nonsteroidal anti-inflammatory drugs (NSAIDs), is frequently detected in municipal and surface waters at concentrations in the microgram per liter (µg/L) range. [1] Due to its chemical stability and resistance to conventional biological treatments, its complete removal from aquatic environments remains a major challenge. [3] The scientific literature describes several effective elimination methods, including adsorption, advanced oxidation processes (AOPs), photocatalysis, and membrane separation techniques. [2,4]*

Adsorption is considered one of the most efficient and cost-effective methods for ibuprofen removal from water. [1] Common adsorbents include activated carbon, modified biochar, graphene oxide, and metal-organic frameworks (MOFs). Reported maximum adsorption capacities range between 100 and 250 mg/g, depending on the surface area and chemical functionalization of the material. [4] Optimal working parameters are typically at pH 4–5, where ibuprofen exists predominantly in its neutral form, enhancing hydrophobic and π–π interactions. Temperature increases (25–40 °C) generally improve adsorption kinetics due to higher diffusion rates. [5]

Advanced oxidation processes (AOPs) rely on the generation of hydroxyl radicals (•OH) with a high oxidation potential (E° = 2.8 V), capable of completely mineralizing organic pollutants. [4] Among the most studied AOPs are the photo-Fenton and electro-Fenton processes. In the classical Fenton reaction, the Fe^{2+}/H_2O_2 system generates radicals according to the mechanism: $Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH^- + \bullet OH$. [1] The photo-Fenton variant introduces UV or visible light irradiation, which regenerates Fe^{2+} ions and accelerates degradation rates. Optimal operational conditions include pH 2.8–3.0 (to prevent Fe precipitation) and an $Fe^{2+}:H_2O_2$ molar ratio of 1:10. Under these conditions, degradation efficiencies above 95% for ibuprofen have been reported within 30–60 minutes of reaction time. [3,5]

Other complementary methods include ozonation, which produces reactive oxygen species that transform ibuprofen into more biodegradable intermediates, and membrane processes (nanofiltration, reverse osmosis), which achieve physical retention above 85%. [1] Emerging approaches such as bio-Fenton hybrid systems integrate biological degradation with oxidative steps, aiming to enhance sustainability and minimize chemical consumption.[2]

In conclusion, the removal of ibuprofen from water requires an integrated approach. Adsorption provides an efficient, rapid, and reusable technique, while advanced oxidation ensures complete mineralization of persistent residues.[1] Hybrid systems combining adsorption and photo-Fenton oxidation have shown the highest overall efficiency (>95%) under controlled pH and temperature conditions. Implementing these technologies at a full scale represents a key step toward reducing ecotoxicological risks and protecting aquatic resources. [2,5]

Key Words: water treatment, Ibuprofen, advanced oxidation processes, photo-Fenton, adsorption, membrane filtration, ozonation

* Corresponding author: florina.lungu@stud.chimie.upb.ro

* Corresponding author: daniela.stefan@upb.ro

References:

[1] Silva CP, Lima DL, et al. Removal of pharmaceuticals by advanced oxidation processes. Chem Eng J.2017;318:608–20.
[2] Ayati A, et al. Ibuprofen adsorption using carbon-based materials. J Environ Chem Eng. 2019;7:103–118.
[3] Kumar M, et al. Emerging contaminants and treatment strategies. Sci Total Environ. 2020;714:136–148.
[4] Loaiza-Ambuludi S, et al. Ibuprofen degradation by photo-Fenton. Appl Catal B. 2015;180:44–52.
[5] Meghea I, et al. An integrative approach to hazardous effects caused by pharmaceutical contaminants on aquatic effluents. Molecules. 2025;30:3483. https://doi.org/10.3390/molecules30173483

SA-P20 ARTIFICIAL NEURAL NETWORK MODELLING FOR THE PREDICTION OF WWTP EFFLUENT ORTHO-PHOSPHATES CONCENTRATION

Tudor M. Chiciudean[1], Norbert B. Mihaly[1,*], Nicolae Cebotaru[1,2], Marius A. Brehar[1,2], Radu Cauacean[2], Elisabeta C. Timis[1]

[1]Department of Chemical Engineering, Babeș Bolyai University, 11 Arany János Street, 400028 Cluj-Napoca, Romania
[2]Compania de Apa Somes SA, Cluj-Napoca, Romania

Abstract: *This paper presents a neural network model to predict the effluent ortho-phosphates concentration in the Cluj-Napoca wastewater treatment plant. The model may be further used for monitoring (i.e., none or faulty hard sensors) and process control purposes*.
Key words: wastewater treatment, data driven model, artificial neural networks, phosphorus.

Introduction: As an important indicator for the eutrophication of rivers, the accurate prediction of ortho-phosphates concentration is crucial for the Wastewater Treatment Plant (WWTP) control strategy.[1] Artificial neural networks (ANNs) take into account the high time correlation between WWTP data and their nonlinear mapping ability.[2] Therefore, ANNs are widely used to characterize the complexity of WWTPs.

Experimental and Modelling: The data used for the ANN model development and independent testing was collected from the Cluj-Napoca WWTP (maximum capacity of 111,000 m^3/day) over a period of 15 days, at a frequency of 10 s. It was then reduced to 10 minutes intervals by averaging every 60 points. Normalized values were randomly divided into 3 sets: 80% for training, 10% for testing and 10% for validation. The ANN architecture was developed using the trial-and-error methodology, until a satisfactory result was achieved.

Results and discussions: The ANN model has an architecture of 2 hidden layers (15 and 10 neurons; logistic sigmoid function) and an input delay of 46 previous moments (7.66 hours). Its performance assessment, using multiple indicators, reveals very good results on the testing data: the coefficient of determination (R^2: 0.921), the root mean squared error (RMSE: 0.0045) and the mean absolute percentage error (MAPE: 2.0722).**Error! Reference source not found.**The analysis of ANN predictions against WWTP measurements revealed excellent model behavior in following the process dynamics (Fig. 1) and a symmetrical distribution of model outputs along the targets line (Y = T in Fig. 2). This indicates no bias tendency or systematic errors in any direction. Simulation results validate

* Corresponding author: norbert.mihaly@ubbcluj.ro

the precision and accuracy of the ANN model as a soft sensor and support its further use as a process monitoring support tool.

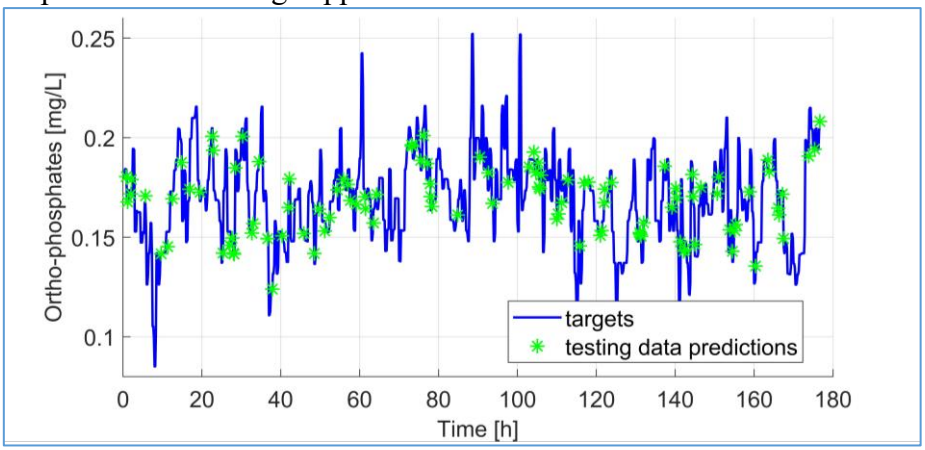


Fig. 1 Model results against measurements for the testing data: ortho-phosphates dynamics.

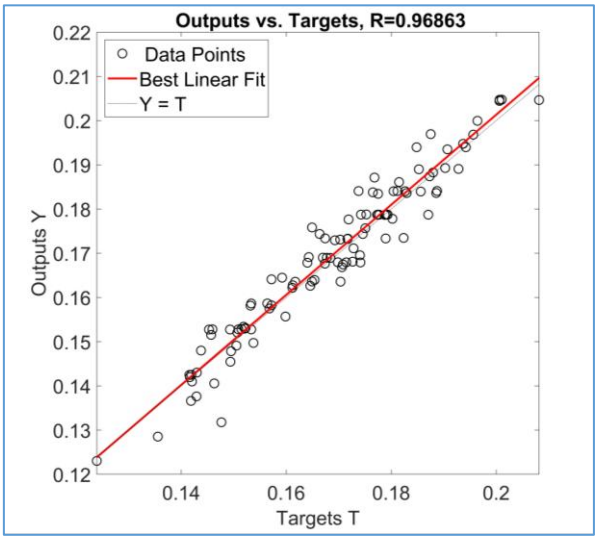


Fig. 2 Model results against measurements visualized for the test data: ANN regression plot.

Conclusions: An accurate ANN model for ortho-phosphates concentration in the effluent has been developed and verified against field data from the Cluj-Napoca WWTP.

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0666, within PNCDI IV.

References:

[1] Wenjing L., Zhigang L., Junfei Q., DEPFSWNN: A data-driven efficient pruning feedforward small-world neural network as a virtual sensor for total phosphorus in wastewater treatment process. Expert Syst. Appl., 296 B, (2026), 129007.

[2] Pisa I., Santín I., Morell A., Lopez Vicario J., Vilanova R., LSTM-Based Wastewater Treatment Plants Operation Strategies for Effluent Quality Improvement. Advanced Sensor Technologies on Water Monitoring and Modeling, IEEE Access 7, (2019), 159773–159786.

SA-P21 SIMULATION OF FIXED-BED REACTOR FOR COPPER-BASED CHEMICAL LOOPING

Levente Biró[1], Ana-Maria Cormoș[1,*]

[1]Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, 11 Arany János, 400028, Cluj-Napoca, Romania

The critical challenge in controlling global warming is finding highly efficient CO_2 capture methods. Chemical Looping Combustion (CLC) is a leading candidate, but its successful implementation depends on precise kinetic and operational models of its fundamental processes. This work focuses on developing and validating a robust mathematical model for the regeneration (oxidation) step of the copper-based oxygen carrier (OC) within a fixed-bed reactor (FiBR) system. The schematic flowsheet diagram of the simulated CLC reactor is illustrated by *Figure 1*. [1,2].

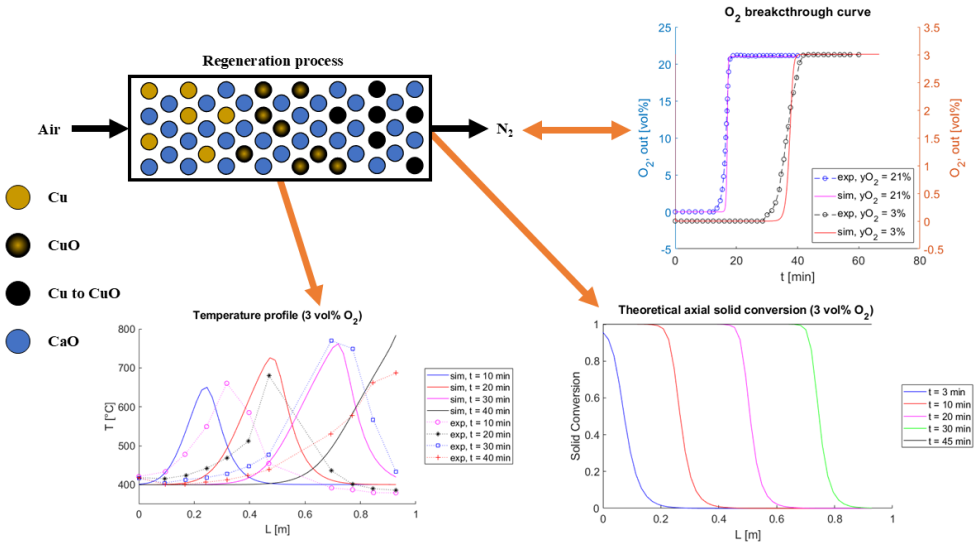


Figure 1. – Schematic flowsheet diagram of the modelling process.

The research goal is to develop an accurate model of the oxidation process, of Chemical Looping Combustion system, where the OC material is generated from Cu metal. During the modeling of the process various gas feeds and O_2 concentrations were assessed. However, the model of the CLC process is described with mass- and energy balance equations. The partial differential equations of the developed model are discretized, and implemented in Matlab/Simulink, for process simulation. The modeling results are validated by experimental data published by

* Corresponding author: ana.cormos@ubbcluj.ro, levente.biro@ubbcluj.ro

F. García-Labiano *et. al*, and the validation of the operational parameters was performed based on the scientific work of J. M. Alcarón *et. al* [3,4]. In order to create an accurate model, multiple crucial factors are calculated by statistics. The process kinetics are also validated by experimental data.

The next step of the development is to improve the model of the reduction process, where the OC material reacts with the fuel and generates CO_2, which needs to be captured. At the end of the research, the developed model needs to include a CO_2 capture unit, powered by CaO to create a Chemical Looping unit with Integrated Combustion and CO_2 Capture system (CL-ICCC).

Keywords: Cu oxidation, Chemical Looping Combustion, Fixed-Bed Reactor, Mathematical modeling, Statistical evaluation

Acknowledgement: This work was supported by a grant from Foundation „Sapientia Hungariae" (Hungary), through the „Collegium Talentum" Scholarship Program.

References:

[1] C. Beuttler *et al.* The Role of Direct Air Capture in Mitigation of Anthropogenic Greenhouse Gas Emissions. *Front. Clim.,* **2019**, *1*,1-10.

[2] H. A. Alalwan *et al.* CO_2 capturing methods: Chemical lopping combustion (CLC) as a promising technique. *Sci. Total Environ.,* **2021**, *788*, 147850-147865.

[3] F. García-Labiano *et al.* Reduction and Oxidation Kinetics of a Copper-Based Oxygen Carrier Prepared by Impregnation for Chemical-Looping Combustion. *Ind. Eng. Chem. Res.*, **2004**, *43*, 8168-8177.

[4] J. M. Alarcón *et al.* Study of a Cu-CuO Chemical loop for the calcination of $CaCO_3$ in fixed bed reactor. *Chem. Eng. J.,* **2017**, *325,* 208-220.

SA-P22 MASS TRANSFER OF INDOLE 3-ACETIC ACID IN A LIQUID MEMBRANE SYSTEM

Roxana Jidveian, Oana Cristina Pârvulescu, Ioana Diaconu, Sorina Laura Topală*

[1]National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnology, 1-7 Gheorghe Polizu St., 011061 Bucharest, Romania

Abstract: *An experimental study and modelling of the separation of indole 3-acetic acid (IAA) from a dilute aqueous solution using chloroform as an organic solvent in the bulk liquid membrane (BLM) phase and trioctylamine (TOA) as a carrier were presented.*
Key words: bulk liquid membrane (BLM); indole 3-acetic acid (IAA); kinetic model; mass transfer; pertraction; trioctylamine (TOA).

Introduction: IAA, the main auxin in plants, has an important role in germination, growth, and development [1]. The pertraction process through a BLM using a suitable carrier (C) is an effective technique applied for the selective separation and concentration of IAA from dilute aqueous solutions [1]. This process involves the following steps: (i) complexation reaction between IAA and C at the interface between the feed (F) and BLM phases; (ii) diffusion of the IAA-C complex through the BLM phase; (iii) decomplexation reaction between the IAA-C complex and stripping agent at the interface between the BLM and stripping (S) phases [1].
Experimental and modeling: The mass transfer of IAA from an aqueous solution using a chloroform BLM and TOA as a carrier was conducted in a tube-in-tube device described in our previous papers [1,2]. The outer tube contained the F phase (an aqueous solution of IAA) at the top and the BLM phase at the bottom, whereas the inner tube contained the S phase (an aqueous solution of NaOH). Ten experimental runs were performed at different levels of process factors, *i.e.*, initial molar concentrations of IAA in the F phase ($c_{IAA,F0}$ = 10^{-4}–10^{-3} mol/L) and NaOH in the S phase ($c_{NaOH,S0}$ = 10^{-2}–1 mol/L). Each test was carried out for 4 h, under mechanical stirring of inner tube (200 rpm), at the room temperature, and at an initial molar concentration of TOA in the BLM phase ($c_{TOA,BLM0}$) of 10^{-2} mol/L. It was assumed that the F, BLM, and S phases were perfectly mixed and their volumes remained constant during the process (V_F = 20 cm^3, V_{BLM} = 50 cm^3, and V_S = 7 cm^3). Specific amounts of IAA in the F, S, and BLM phases (R_F, R_S, and R_{BLM}), which are defined by equations (1)–(3) [2], were selected as response variables. The molar concentrations of IAA in the F and S phases ($c_{IAA,F}$ and $c_{IAA,S}$) were measured every 30 min using a spectrophotometer (UV1900i, Shimadzu, Kyoto, Japan). A kinetic model based on consecutive irreversible first-order reactions was used to predict the specific amounts of IAA in the membrane system phases ($R_{F,pred}$, $R_{BLM,pred}$, and $R_{S,pred}$), which are defined by equations (4)–(6) [2]. The kinetic parameters of the

* Corresponding author: maholealaura@yahoo.com

model, *i.e.*, extraction and stripping rate constants (k_1 and k_2), were regressed from the experimental data. The maximum final values (at 4 h) of extraction, stripping, and recovery efficiencies (E_{Ef}, E_{Sf}, and E_{Rf}) were calculated using equations (7)–(9) [2].

$$R_F = \frac{c_{IAA,F}V_F}{c_{IAA,F0}V_F} = \frac{c_{IAA,F}}{c_{IAA,F0}} \quad (1)$$

$$R_S = \frac{c_{IAA,S}V_S}{c_{IAA,F0}V_F} \quad (2)$$

$$R_{BLM} = \frac{c_{IAA,BLM}V_{BLM}}{c_{IAA,F0}V_F} = 1 - R_F - R_S \quad (3)$$

$$R_{F,pred} = e^{-k_1 t} \quad (4)$$

$$R_{BLM,pred} = \frac{k_1}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) \quad (5)$$

$$R_{S,pred} = 1 - R_{F,pred} - R_{BLM,pred} = 1 - \frac{1}{k_2 - k_1}\left(k_2 e^{-k_1 t} - k_1 e^{-k_2 t}\right) \quad (6)$$

$$E_{Ef} = 100\left(1 - \frac{c_{IAA,Ff}}{c_{IAA,F0}}\right) = 100\left(1 - R_{Ff}\right) \quad (7)$$

$$E_{Sf} = \frac{100 c_{IAA,Sf}V_S}{(c_{IAA,F0} - R_{Ff}c_{IAA,F0})V_F} = 10000\frac{R_{Sf}}{E_{Ef}} \quad (8)$$

$$E_{Rf} = 100\frac{c_{IAA,Sf}V_S}{c_{IAA,F0}V_F} = 100R_{Sf} = \frac{E_{Ef}E_{Sf}}{100} \quad (9)$$

Results and conclusions: The values of kinetic parameters were similar, suggesting that both chemical reactions of complexation and decomplexation were rate-limiting steps. A good agreement between experimental and predicted data (R^2 = 0.968–0.995) was obtained. The maximum final value of R_S (R_{Sf} = 0.924), corresponding to the maximum values of E_{Ef} (95.00%), E_{Sf} (97.26%), and $E_{Rf,ex}$ (92.40%) were obtained at $c_{IAA,F0} = 10^{-4}$ mol/L and $c_{NaOH,S0} = 1$ mol/L.

The pertraction process through a chloroform BLM using TOA as a carrier is a simple, inexpensive, and effective technique applied for separation and concentration of IAA from dilute aqueous solutions.

Acknowledgments: This work was supported by a grant from the National Program for Research of the National Association of Technical Universities – GNAC ARUT 2023 (128/04.12.2023).

References:

[1] Diaconu, I., Pârvulescu, O. C., Topală, S. L., Dobre, T., Effects of process factors on performances of liquid membrane-based transfer of indole-3-acetic acid, *Scientific Reports*, 11, 1, (2021), 23427.

[2] Diaconu, I., Pârvulescu, O. C., Badea, G. I., Rotaru, M., Orbeci, C., Cernica, G., Use of bulk liquid membranes for the removal of aspartame from aqueous media, *Journal of Molecular Liquids*, 409, (2024), 125456.

SA-P23 ELECTRICITY PRODUCED FROM THE RECOVERY OF ORGANIC WASTE IN A MEAN SIZE AGRICULTURAL HOLDING

Anca Mădălina Dumitrescu and Paula Postelnicescu

National University of Science and Technology Politehnica Bucharest

Abstract: *The paper presents an applied technological study regarding the production of biogas and its subsequent use to produce electricity, at the level of an average size farm.*
Key words: biogas, anaerobic fermentation.

Introduction: One of the most effective methods for recovering energy from agricultural organic waste is anaerobic fermentation at elevated temperatures [1]. This process is highly efficient for converting solid and liquid organic materials—such as animal manure and plant biomass—into non-conventional energy sources. Anaerobic fermentation can be replicated in sealed systems known as anaerobic digesters. Within these digesters, microorganisms break down organic matter in the absence of oxygen, producing a range of fermentation byproducts. The primary gaseous outputs are carbon dioxide (CO_2) and methane (CH_4), with methane being the dominant component. This methane-rich biogas serves as a valuable renewable energy source, contributing to sustainable waste management and energy production. The use of the biological mass potential generated by anaerobic digestion within a rural ecological deposit, its transformation into biogas together with the avoidance of pollution represents a current strategic option and at the same time, a technical solution for the future [2].

Modeling: The calculations were made for an agricultural holding with a 150 cows farm and a 250 animals piggery. Average dropping and dirt quantity per month are known, and there is a problem concerning their storage and removal. As a solution, they will be used to provide biogas by anaerobic digestion. To correctly calculate the ratio between animal dropping and agricultural vegetal remains it is necessary to provide a carbon/nitrogen ratio in the domain 20 – 30. In this paper, the following composition of the raw materials was proposed: bovine manure 3 parts, swine manure 3 parts, corn cobbs 1part, straw 1 part, vegetable remains 2 parts. For this composition the carbon/nitrogen ratio is 29.6.

The biogas yield obtained $Biogas\ yield = \frac{V_{biogas}}{M} = \frac{4.88 \cdot 10^4}{142.027} = 343.5\ m^3/t$

The calorific value of biogas (LHV) is 18–26 MJ/m^3 (on average, about 6 kWh/m^3).

Results: Considering that the average electricity consumption for a rural household is 2.4 MWh, the quantity of biogas obtained from the farm waste can be used by approximately 900 dwellings.

To ensure sustainable use of biogas energy, it is essential to promote its production through targeted investments and technological advancements, while simultaneously stimulating demand by implementing policies that incentivize biogas consumption.

References

[1] T. Tutunaru, ”Producerea biogazului şi valorificarea lui în scopuri energetice”, Meridian Ingineresc, 1, 2009, 62-67, ISSN 1683-853X; **[2]** M. J. B. Kabeyi, O. A. Olanrewaju, ”Biogas production and applications in the sustainable energy transition”, Hindawi, Journal of Energy, Volume 2022, Article ID 8750221, 43 pp. https://doi.org/10.1155/2022/8750221

SA-P24 ANALYSIS OF TWO-PHASE FLOW IN A COUNTER-CURRENT BUBBLE COLUMN AS A FUNCTION OF OPERATING PARAMETERS: AN EXPERIMENTAL INVESTIGATION OF GAS AND LIQUID VELOCITIES

Adib Essid[1,*], Jean-Pierre Fontaine[1], Alina-Violeta Ursu[1], Christophe Vial[1]

[1]Université Clermont Auvergne, CNRS, Clermont Auvergne INP, Institut Pascal, F-63000, Clermont-Ferrand, France, adib.essid@uca.fr

Abstract: *The hydrodynamics of a counter-current bubble column designed to simulate a biological methanation process was investigated. The study focused on the measurement of local gas and liquid velocities under different operating conditions using high-speed imaging techniques. Measurements were carried out at multiple axial positions within the column. The results showed that both local gas and liquid velocities are strongly influenced by the operating parameters, especially at higher superficial flow rates. Furthermore, the gas velocity profiles exhibit pronounced heterogeneity along the reactor axis, reflecting the presence of complex flow and recirculation structures, whereas the liquid velocity remains comparatively uniform, suggesting a more homogeneous continuous phase.*

Keywords: bubbly flow, hydrodynamics, local gas velocity, local liquid velocity, bubble column

Introduction: As part of energy transition green methane is increasingly produced by catalytic methanation or biological methanation [1]. While the biological route benefits from milder operating conditions (lower temperature and pressure) its performance is frequently mass transfer limited due to the low solubility of H_2 gas in aqueous media [2]. Therefore, this work investigates a counter-current bubble column for methane production by high-speed imaging techniques, assessing how the operating parameters affect the local hydrodynamics.

Materials and methods: Experiments were carried out in pure water, used as a representative model medium for biomethanation culture media. The experimental setup consisted of a custom-built countercurrent flow 3-L bubble column made of a transparent PVC cylinder (54 mm internal diameter, 1400 mm height). A transparent water-filled box (0.15×0.12 m^2) able to move on the column axis, was designed to reduce optical distortion. The air network was supplied using a mass flow controller (3) (Bronkhorst, USA). The bubbles were created using a sintered ceramic sparger with a porosity of 10 to 16 μm (5). The gas flow rate (Q_g) varied between 3 and 12 $L.h^{-1}$. The downward liquid flow was imposed using a peristaltic pump (M6-6L, headed DZ25-6L, Innofluid Co., China) (4) with a liquid flow rate (Q_l) in the range 0 - 144 $L.h^{-1}$. Gas phase velocity (in the *xy* plane) was obtained by back-lit high-speed imaging using a camera (Kron Technol. Inc., Canada) and a LED panel to capture bubbles on a white background (1280×1024 $pixels^2$, 1069 fps) software was used to extract the 2D bubble velocity components from the videos using Tractrac PTV [3]. For the liquid phase, planar PIV (*2D2C)* technique was used to measure the velocity of the liquid in the *xy* plane. A laser sheet was generated with an MGL-N 4 W, 532 nm laser (Dantec Dynamics SA, Denmark) to illuminate seeding particles (S-HGS for single-phase flow; PMMA-RhB for two-phase flow), and images were acquired with the same camera as above. The raw images were processed using PIVLab 2.63 software [4]. To access the out-of-plane

component, stereoscopic PIV *(3C-2D)* was employed in the same laser sheet (pulsed mode) and the same seeding particles, but with two high-performance cameras (IDS, UI-3060CP, resolution: 1936x1216 pixels). The raw images were processed using Hiris software (R&D vision, France) to determine 2D velocity components (*Vx*, *Vy*), and the *Vz* component was reconstructed using a StereoPIV software (R&D vision, France). Three measurement areas regions were defined.

Results and Discussion: Figures 1 and 2 display gas and liquid velocity data for various Q_g and Q_l. At low Q_g, the gas phase velocity field is heterogeneous, with lower velocities in the reactor core and higher velocities occurring near the walls. As Q_g increases, the velocity profile becomes more uniform and the bubble upward velocity increases. This trend is consistent with a spatial bubble size distribution, with larger bubbles preferentially located close to the walls and small bubbles in the core region. Figure 1 shows that liquid recirculation, for $Q_l \geq 72$ L.h^{-1}, opposes bubbles rise, thereby reducing bubble velocity and increasing their bubble residence time in the reactor. In two-phase flows, the liquid velocity profile typically features two distinct regions: a low-velocity zone where bubbles rise counter-currently to the liquid, and a high-velocity zone characterized by low gas hold-up and a downward liquid flow. The 2D liquid velocity profiles obtained from *2D2C* PIV and SPIV are in close agreement, supporting the accuracy of the measured in-plane components *Vxy*. The 3D liquid velocity data shows that the gas phase induces non-negligible V_z values due to bubble-driven out-of-plane motion and local flow deflection. Furthermore, the gas phase velocity exhibits axial heterogeneity, which decreases from the sparger region to the top of the column. This trend is consistent with the radial dispersion of the bubbles.

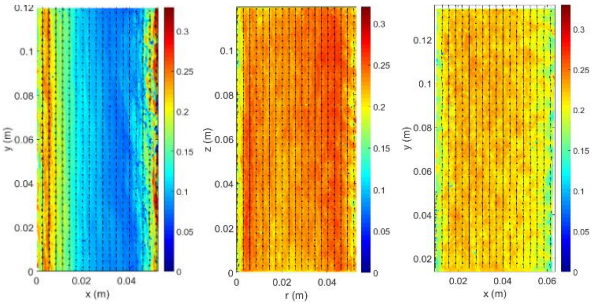


Figure 1: Gas velocity at (a) Q_g=3 l/h and Q_l=0 l/h, (b) Q_g=12 l/h and Q_l=0 l/h, (c) Q_g=12 l/h and Q_L=144 l/h.

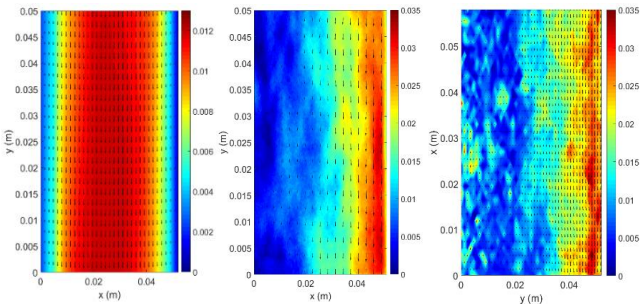


Figure 2: Liquid velocity: V_{xy} at (a) Q_g=0 l/h and Q_l=72 l/h, (b) Q_g=9 l/h and Q_l=72 l/h; (c) V_{xyz} at Q_g=9 l/h and Q_l=144 l/h.

Conclusion: The local velocity field of both phases exhibit a strong dependence on operating parameters. Within the investigated range of gas flow rate, an optimum range of liquid counter-current flow can be identified to improve hydrodynamics and mass transfer at low power input.

References: **[1]** Leonzio G., *Chem. Eng. J.* 290, 490-498 (2016).; **[2]** Lecker B., Illi L., Lemmer A., Oechsner H., *Biores. Technol.* 245A, 1220-1228 (2017). ; [3] Heyman J., TracTrac: *Comput. Geosci.* 128, 11–18 (2019).; [4] Thielicke W., Sonntag R., *Journal of Open Research Software* 9, 1-14 (2021).

SA-P25 SUSTAINABLE DOWNSTREAM PROCESSING IN BIOREFINERIES OF PHOTOSYNTHETIC AQUATIC MICROORGANISMS

Alina-Violeta Ursu[1, *], Philippe Michaud[1], Christophe Vial[1], Alain Marcati[1], Gholamreza Djelveh[1],

[1] Clermont Auvergne Université, Clermont Auvergne INP, CNRS, Institut Pascal, Clermont-Ferrand, F-63000, France

Abstract: Photosynthetic aquatic microorganisms including eukaryotic microalgae and cyanobacteria, offer a versatile reservoir of renewable, high-value biomolecules for applications in bioenergy, food, cosmetics, and health [1]. However, algal biofuels remain economically challenged, with production costs ~3.5–5 times higher than petroleum diesel and still above conventional biofuels; moreover, improved unit economics alone do not ensure environmental or social sustainability [2,3]. Market signals nonetheless confirm growing interest: the global microalgae market was valued at USD 955.1 million (2021), with forecasts reaching USD 1.565 billion by 2030. Among promising genera for proteins and energy carriers (biogas, bioethanol, biodiesel), *Arthrospira* and *Chlorella* dominate, while pilot-scale demonstrations under a biorefinery framework remain comparatively scarce. Notably, the first industrial-scale microalgae biorefinery was established in France in 2025 (SCALE Program), marking a milestone in the maturation of the field. This reality reinforces the biorefinery paradigm: rather than targeting lipids only, microalgal and cyanobacterial biomass-also rich in proteins and carbohydrates-should be processed to co-recover multiple products (fuels, energy carriers, chemicals) so that aggregate market value can exceed production costs within a sustainability framework.

Advancing an integrated and sustainable biorefinery requires: *(i)* discovery of novel bioactives; *(ii)* optimizing solid–liquid extraction and purification for yield, energy demand, and environmental footprint; *(iii)* circular valorisation of co-products (bioCH_4, bioH_2, ethanol, volatile fatty acids) toward energy-neutral/positive operations; and *(iv)* predictive structure–property/activity modelling. A critical downstream priority is cell disruption, tailored to cell-wall architecture, as it conditions extraction efficiency. Altogether, sustainable downstream bioprocessing provides a credible pathway to a circular bioeconomy and low-carbon value chains.

This study compares three photosynthetic aquatic microorganisms, namely two microalgae (*Chlorella vulgaris* and *Porphyridium cruentum*) and one cyanobacterium (*Arthrospira platensis*), to optimize downstream processing steps, with special emphasis on cell wall disruption as dictated by cell wall architecture and on biomolecules with techno-functional applications (e.g., emulsification, foaming).

Keywords: microalgae, cyanobacteria, sustainable biorefinery, downstream processing, cell disruption.

References

[1]. Narayanan M., *Renew. Sustain. Energy Rev*., 190 (B), 114081 (2024).
[2]. Chisti Y., *Biotechnol. Adv.*, 25(3), 294-306 (2007).
[3]. Sunday Okeke E. et al., *Energy Convers. Manag., 16,* 100323 (2022).

* Corresponding author: alina_violeta.ursu@uca.fr

BOOK OF ABSTRACTS

SICHEM – 2025

B – Applied organic, inorganic, and supramolecular chemistry in process engineering (AOISCPE)

1. Keynotes

SB-KN01 THE USE OF AUTOMATIC PROCESS DEVELOPMENT FOR OPTIMIZATION OF CRITICAL PROCESS PARAMETERS IN VARIOUS DRUG SYNTHESES

Cristian Condeiu[1]*, Gherghina Ciortan[2]

[1] Lewis University, One University Dr, Romeoville, IL 60446, USA

[2]CEPROCIM, SA, #6, Preciziei Blvd, Sector 6, Bucharest, 062203

***Abstract**: Automated Process Development (APD) allows gathering essential decision-making data with minimal costs of material and time. APD facilitates Quality by Design (QbD) as a systematic approach to development that begins with predefined objectives. One of the APD goals is to determine critical parameters (Critical Quality Attributes) in a minimal number of experiments, using Design of Experiments (DOE). The present paper describes two case studies using APD to determine optimal parameters for maximum yields. Optimization of reaction conditions used Ease Design-Expert developed by StatEase as DOE software. The experiments used robotic equipment such as Resonant Acousting Mixing (RAM) unit fitted with 48-reactor blocks, Gilson liquid dispensers, Bohdan weighing station and Gilson high-throughput liquid chromatography system. The first case study focused on the optimization of the synthesis of a heterocyclic compound, leading to optimal synthesis conditions regarding reaction temperature and the molar ratio between reactants. The second case study aimed at optimizing the parameters of a Friedel–Crafts acylation reaction, identifying the best solvent and Lewis acid, as well as the optimal reaction temperature and optimal amount of Lewis acid.*

The APD approach is based, like any optimization, on a mathematical model that involves finding the objective function and the restrictive function. The objective function is the mathematical expression of the quantitative influence of the most significant parameters on the quality characteristic of the reaction system. The restrictive function is the function that defines the permissible range of variation for the objective function and the parameters of the reaction system. In conclusion, finding the optimal conditions for carrying out a chemical reaction means identifying the conditions corresponding to the maximum or minimum of the objective function, which must be thoroughly studied using analytical or alphanumeric optimization methods. In practice, optimization problems can be solved with the help of statistical methods such as factorial experiments and analysis of variance. An analytical system with functions of detection, identification, or determination is an informational chain in which the material to be analyzed (sample) is the input, and the analysis result is the output, as presented in the two case studies.

APD represents a highly useful approach for optimizing reaction parameters for virtually any type of chemistry, with applications in process development/optimization.

Keywords: automated process development, optimization of reaction conditions, robotic equipment, design of experiments, mathematical model, objective function, restrictive function

Introduction: APD found multiple applications in the synthesis of peptides [1], nucleic acids [2], and polysaccharides [3]. However, one of the main applications of APD remains determination of optimal reaction conditions, using the principles of Design of Experiments (DOE) to maximize yield or minimize side products and production costs, such as in the optimization of reaction conditions for heteroaryl Suzuki-Miyaura coupling [4]. Robotic equipment is very often used. Advantages of APD are significant decrease in research time by simultaneous exploration of multiple sets of reaction conditions, and use of minimal

* Corresponding author: condeich@lewisu.edu

amounts of raw materials to generate minimal waste. Two case studies involving heterocycles are described.

Experimental: *Equipment:* Resonant Acousting Mixing (RAM) unit fitted with 48-reactor blocks, Gilson liquid dispensers, Bohdan weighing station and Gilson high-throughput liquid chromatography systems. DOE software used in the optimization of reaction conditions was Ease Design-Expert developed by StatEase.

Reagents: all reagents used were either ACS-grade or obtained from ACS grade.

Reaction conditions were evaluated at different temperatures, molar ratios between reactants, and quantities of catalyst, and different solvents and catalysts were tested to determine the best yield.

Results and discussions: for the synthesis of 4,5-disubstituted imidazoles, best yields were obtained at temperatures of 155°C–165°C and molar ratios formamide:bromoacetone of 8.0:9.5.

Acylation reaction leading to a coumarine derivative produced best yields with nitromethane as solvent and $AlCl_3$ as catalyst, at a temperature of 90°C and using 5.5 eq. $AlCl_3$.

DOE used in reaction planning was based on a mathematical model that involved finding the objective function and the restrictive function [5].

Conclusions: APD is a very useful approach in optimizing reaction parameters. It leads to optimal reaction conditions in much less time and number of experiments. Regardless of the method used for establishing the optimum, an optimum may exist either as stationary point, or as point of discontinuity, or as point of margin.

References:

[1] R. B. Merrifield, Automated synthesis of peptides, Science 150, 178–185 (1965).
[2]. M. H. Caruthers, Gene synthesis machines: DNA chemistry and its uses, Science 230, 281–285 (1985).
[3] O. J. Plante, E. R. Palmacci, P. H. Seeberger, Automated solid-phase synthesis of oligosaccharides, Science 291, 1523–1527 (2001).
[4] Angello et al., Closed-loop optimization of general reaction conditions for heteroaryl Suzuki-Miyaura coupling, Science 378, 399–405 (2022)
[5] J.CEA, Optimization-theory of algorithms, Dunnod, Paris, 1971

BOOK OF ABSTRACTS

SICHEM – 2025

B – Applied organic, inorganic, and supramolecular chemistry in process engineering (AOISCPE)

2. Oral presentations

SB-OP01 LOW-TEMPERATURE ETHANE OXYDEHYDROGENATION OVER M-MODIFIED (M = Sn, Ti, Sb, Ta) NiNbO MIXED OXIDE CATALYSTS

Ştefan-Bogdan Ivan[1], Ionel Popescu[2], Cătălin Negrilă[3], Florica Papa[4], Stéphane Loridant[5], Ioan-Cezar Marcu[1,*]

[1] Faculty of Chemistry, University of Bucharest, 030018 Bucharest, Romania

[2] Division of Exact Sciences, Research Institute of the University of Bucharest, 050663 Bucharest, Romania

[3] National Institute of Materials Physics, 077125 Măgurele, Romania

[4] "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 060021 Bucharest, Romania

[5] Université Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, 69100, France

Abstract: *New M-NiNbO mixed oxide catalysts with M = Sn, Ti, Sb and Ta were prepared by hydrothermal and solvent evaporation methods, characterized using a battery of techniques and evaluated in low-temperature ethane oxydehydrogenation.*
Key words: Ethane, Ethylene, Oxydehydrogenation, Nickel Niobium Oxide Catalyst, Promoters

Introduction: Low-temperature catalytic ethane oxydehydrogenation (ODH) is an attractive alternative to the conventional steam cracking route for ethylene production. $Ni_{0.85}Nb_{0.15}O$ mixed oxide was found to be a highly efficient catalyst for this reaction [1]. However, it loses partially its activity but gains a high selectivity to ethylene over time on stream [2]. In the present work, this catalytic system was modified with tetravalent (Sn, Ti) and pentavalent (Sb, Ta) cations in order to improve its performance.

Experimental: *Catalysts preparation:* $Ni_{0.85}Nb_{0.15}O$ and $(NiNb)_{0.9}M_{0.1}O$ mixed oxides, labeled NiNbO and M-NiNbO, with M = Sn, Ti, Sb and Ta, and the Nb/Ni atomic ratio set to 0.176, were prepared by hydrothermal and solvent evaporation methods [3]. Additionally, $(NiNb)_{0.9}Ta_{0.1}O$ and $(NiNb)_{0.95}Ta_{0.05}O$ mixed oxides, labeled Ta-NiNbO-8 and Ta(5)-NiNbO-8, were prepared by the hydrothermal method at basic pH of 8. All the catalysts were calcined at 450 °C under air. *Catalysts characterization:* Several techniques, including XRD, SEM-EDX, XPS, H_2-TPR, MicroRaman and *in situ* electrical conductivity measurements, were used to characterize the catalysts. *Catalytic tests:* Their catalytic properties in ethane ODH were evaluated in a fixed-bed continuous-flow reactor in the temperature range 325-425 °C using an ethane-air mixture. On-stream stability tests for NiNbO and Ta-modified NiNbO catalysts were run up to several dozens of hours at 400 °C.

* Corresponding author: ioancezar.marcu@chimie.unibuc.ro

Results and discussions: Nanometric NiO was the dominant crystalline phase in all the mixed oxides. Amorphous phases were also evidenced in all tricationic oxides. Additionally, SnO_2 was identified in Sn-NiNbO, while an unidentified crystalline phase was observed in both Ta-containing samples prepared at pH of 8. The latter contained both surface Nb^{4+} and Nb^{5+} species, while all other samples contained only surface Nb^{4+}. Both Nb/Ni and M/(Ni+Nb) bulk atomic ratios were close to their theoretical values for all mixed oxides, except for Ta-NiNbO, for which they were noticeably larger. Their surface areas ranged from 52 m^2 g^{-1} for NiNbO to 265 m^2 g^{-1} for Sb-NiNbO. All the catalysts were p-type semiconducting oxides with the positive holes associated to O^- lattice species. These species are able to activate ethane and, when less numerous, to transform it into ethylene. All the catalysts were partially reduced under the reaction mixture, Ta-NiNbO-8 and Ta(5)-NiNbO-8 showing the highest extent of reduction. All the mixed oxides slightly but steadily lost their initial conductivity and redox ability in time.

At 400 °C, the ethane conversion (values in parentheses) followed the order: Ti-NiNbO (21 %) < Sn-NiNbO (36 %) < Sb-NiNbO (37 %) < Ta-NiNbO (45 %) < NiNbO (54 %) < Ta-NiNbO-8 (58 %) < Ta(5)-NiNbO-8 (62 %). Conversion vs selectivity data at 400 °C, allowing comparisons at isoconversion, showed that Ta(5)-NiNbO-8 and Ta-NiNbO-8 were the most selective catalysts in the series, in line with their highest extent of reduction observed under the reaction mixture. With 62 % conversion and 68 % ethylene selectivity at 400 °C, Ta(5)-NiNbO-8 exhibited the best performance in ethane ODH likely due to its lowest O^- lattice species density. Nevertheless, none of the catalysts remained stable over time on stream: the conversion decreased while the selectivity slightly increased. This deactivation was attributed to structural and surface compositional changes of the oxides and also to their gradual loss of p-type conductivity and diminished reoxidation capacity evidenced by electrical conductivity measurements.

Conclusions: The addition of the third cation M (M = Sn, Ti, Sb and Ta) to NiNbO together with the preparation conditions and the content of the modifier have a marked effect on the physicochemical properties of the resulting M-NiNbO tricationic oxides and, hence, on their catalytic performance in ethane ODH. The best catalyst in this series, outperforming the unmodified NiNbO system, was Ta(5)-NiNbO-8 mixed oxide, which gave 42 % ethylene yield at 400 °C. However, none of the catalysts showed long-term stability on stream.

References:

[1] Heracleous E., Lemonidou A.A., Ni–Nb–O mixed oxides as highly active and selective catalysts for ethene production via ethane oxidative dehydrogenation. Part I: Characterization and catalytic performance, *J. Catal.*, 237 (2006) 162-174.

[2] Savova B., Loridant S., Filkova D., Millet J.M.M., Ni–Nb–O catalysts for ethane oxidative dehydrogenation, *Appl. Catal. A*, 390 (2010) 148-157.

[3] Ivan Ş.-B., Popescu I., Negrilă C., Papa F., Loridant S., Marcu I.-C., Effect of modifying NiNbO catalyst with tetravalent (Sn, Ti) and pentavalent (Sb, Ta) cations on its ethane oxidative dehydrogenation performance, *Ind. Eng. Chem. Res.*, 64 (2025) 18692-18712.

SB-OP02 CONSIDERATIONS FOR MODELING, CALCULATION AND AUTOMATION OF A FIRE SUPPRESSION INSTALLATION IN AN INDUSTRIAL FACILITY

Cosmin Guran[1*], Adina Gavrila[1], Oana Parvulescu[1], Timur Chis [2], Dobre Tanase[1]

[1]National University of Science and Technology Politehnica Bucharest, Polizu 1-7, 01161, Bucharest Romania;

[2]Petroleum and Gas University of Ploiesti, B[dul] Bucuresti 39, Ploiesti, Romania

Abstract: *The main purpose of the work is to show how it optimizes fire detection, signaling and extinguishing systems for various installations, so as to minimize the risk of all loss types*
Key words: Industrial warehouse, Suppression fire installation, Computing model

Introduction. The optimizing fire detection, signaling and extinguishing systems for various installations, to minimize the risk of loss of human life and material damage expresses a problem with important legal constraints [1-3]. The main factors that influence this optimization are given by the technical specifications of the construction and are specific to each investment. We will optimize fire detection, signaling and extinguishing systems under the influence of: i) built-up area / area deployed, ii) volume of space, iii) degree of fire resistance, iv) type of technological process or stored materials, v) height regime, vi) maximum height. **Experimental and/or Modelling:** From past experiences we have found that any building can be subject to fire risk, and the best method to save lives, but also to minimize damage caused by a possible fire is taking prevention measures [4]**. Results and discussions.** The dimensioning of the suppression installation presented with this paper represents the optimal system model that reduces to a minimum the possible losses caused by an eventual fire. Some advantages offered by the system are a) Early fire detection, b) 24/7 Protection: Fire detection and suppression systems operate continuously, ensuring permanent monitoring of the protected area. This means they are activated and ready to respond to any sign of fire at any time of day or night, even when there are no people nearby, c) Rapid response and immediate intervention: Once the fire detection system identifies signs of a fire, it automatically activates the suppression system to quickly and efficiently stop or control the fire. This rapid response can minimize damage and save lives. A case study concentrates on the above subjects.

Conclusions: The problem of fire control in an industrial warehouse was completely applied with a study case.

References **[1]** Law no. 10/1995 regarding quality in construction, modified by Law no. 163/2016; **[2]** I9/2015 – Normative for design and execution of sanitary installations; **[3]** STAS 1478/90 – Sanitary installations. Water supply for civil and industrial buildings. Fundamental prescriptions.; **[4]** P118-2/2013 – Normative regarding fire safety of buildings, with subsequent modifications

* Corresponding author: cosmin.guran@yahoo.com

SB-OP03 DETERMINATION OF PHYSICO-CHEMICAL PROPERTIES AND STABILITY ASSESSMENT OF NANOFUELS CONTAINING MULTI-WALLED CARBON NANOTUBES

Andrei Laurentiu Niculae[1,*], Ioan Calinescu[,2], Petre Chipurici[2], Radu Chiriac[1,3]

[1]NUST POLITEHNICA Bucharest, Faculty of Mechanical Engineering and Mechatronics, 313 Splaiul Independentei, 060042, 6st district, Bucharest, Romania

[2]NUST POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, 1-7 Gheorghe Polizu St., 011061, 1st district, Bucharest, Romania

[3]EA7341 CMGPCE of Conservatoire National des Arts et Metiers, Paris, France

Abstract: *The addition of nanoparticles to fuels can modify their physico-chemical properties, although previous studies have not revealed a clear pattern in these variations. In this study, density, viscosity, and stability were evaluated for a commercial B7 diesel fuel blended with 25, 50, and 100 ppm multi-walled carbon nanotubes (MWCNTs), using 5% n-butanol as the solvent. Span 60 surfactant was used for one sample. The impact on density was minimal, while viscosity varied between −2.21% and +2.56%. Dynamic light scattering (DLS) measurements demonstrated good stability for fuels containing 25 and 50 ppm MWCNTs, whereas significant instability was observed at 100 ppm.*

Key words: Nanofuels, Multi-walled carbon nanotubes, Diesel, Stability, Physico-chemical properties, Fuel additives

Introduction: Improving fuel atomization and combustion efficiency while reducing pollutant emissions remains a major challenge for internal combustion engines. The use of nanoparticles as fuel additives is a promising solution because they can induce puffing and micro-explosions, enhancing atomization [1]. Fuel spray development is also influenced by physico-chemical properties, which can be modified by nanoparticle addition [2]. Previous studies [3–11] indicate negligible effects of MWCNT addition on density at ppm levels, with some variations attributed to surfactants or solvents. For viscosity, both increases and decreases were reported, depending on the base fuel and dispersion stability. This study experimentally determined density, viscosity, and stability of nanofuels with different MWCNT concentrations.

Experimental: A commercial B7 diesel fuel was blended with MWCNTs at 25, 50, and 100 ppm. A 5% n-butanol fraction was used as solvent, and Span 60 surfactant was added to one sample. The prepared fuels were labeled B7S5 (base fuel), B7S5C25, B7S5C50, B7S5C100, and B7S5C100-S (with surfactant, 1 wt.% of the butanol fraction). Samples were homogenized using ultrasonic and mechanical mixing. Density was measured with a pycnometer and recalculated at 15 °C and 40 °C. Kinematic viscosity was measured at 40 °C with an Ostwald viscometer. DLS measurements were performed two months after preparation and repeated after ultrasonic redispersion.

* Corresponding author: andrei.niculae@upb.ro

Results and discussions: All fuels exhibited density and viscosity values within SR EN 590:2022 limits. Density variations were minimal due to the low nanoparticle dosage. The presence of butanol reduced viscosity by 9.24% compared to B7. Adding 25 ppm MWCNTs further decreased viscosity by 2.21%. At higher concentrations, viscosity slightly increased (2.77% at 50 ppm and 2.56% at 100 ppm). The use of Span 60 resulted in a 1.99% decrease and lower viscosity dispersion, indicating improved stability for B7S5C100-S. DLS tests confirmed good stability at 25 and 50 ppm and pronounced instability at 100 ppm.

Conclusions: The impact of MWCNT addition on density was negligible, while viscosity was slightly affected depending on concentration. The addition of Span 60 surfactant enhanced stability, as reflected by reduced viscosity dispersion for B7S5C100-S. Stable dispersions were achieved at 25 and 50 ppm, while 100 ppm showed instability. Stability at higher concentrations may be improved by using functionalized nanoparticles or Span 60 surfactant. Future work will address the influence of these nanofuels on spray development, engine performance, and emissions.

References:

[1] H. Zhang, Z. Lu, T. Wang, Z. Che, Micro-explosion of emulsion droplets with nanoparticles at high temperature, International Journal of Heat and Mass Transfer 219 (2024).

[2] K. Kannaiyan, A. AlDosari, R. Sadr, Effects of nanoscale fuel additives on properties and non-reacting spray performance of alternative, conventional and blended jet fuels at elevated ambient conditions, Fuel Processing Technology 208 (2020)).

[3] A.I. El-Seesy, A.K. Abdel-Rahman, M. Bady, S. Ookawara, Performance, combustion, and emission characteristics of a diesel engine fueled by biodiesel-diesel mixtures with multi-walled carbon nanotubes additives, Energy Conversion and Management 135 (2017) 373–393.

[4] N.M. Nachippan, M. Parthasarathy, P.V. Elumalai, A. Backiyaraj, D. Balasubramanian, A.T. Hoang, Experimental assessment on characteristics of premixed charge compression ignition engine fueled with multi-walled carbon nanotube-included Tamanu methyl ester, Fuel 323 (2022).

[5] J.B. Ooi, C.C. Kau, D.N. Manoharan, X. Wang, M.V. Tran, Y.M. Hung, Effects of multi-walled carbon nanotubes on the combustion, performance, and emission characteristics of a single-cylinder diesel engine fueled with palm-oil biodiesel-diesel blend, Energy 281 (2023).

[6] E. Arslan, M. Raşit Atelge, N. Kahraman, S. Ünalan, B.A. Çeper, Examination of the effect on the engine of diesel-nanoparticle mixture with natural gas addition, Fuel 357 (2024).

[7] H. Solmaz, S.M.S. Ardebili, A. Calam, E. Yılmaz, D. İpci, Prediction of performance and exhaust emissions of a CI engine fueled with multi-wall carbon nanotube doped biodiesel-diesel blends using response surface method, Energy 227 (2021).

[8] B. Ittoo, J.B. Ooi, M.V. Tran, F. Jaliliantabar, G. Hasan Najafi, V. Swamy, Effects of dispersed multiwalled carbon nanotubes on the micro-explosion and combustion characteristics of 2-methylfuran – diesel mixture droplets, Fuel 316 (2022).

[9] R.L. Krupakaran, G.J. Rani, P. Anchupogu, G.V. Reddy, D.R. Reddy, R.K. Petla, Comparative assessment of MWCNTs and alumina nanoparticles dispersion in biodiesel blend on the engine characteristics of an unmodified DI diesel engine, Materials Today: Proceedings 68 (2022) 1241–1251.

[10] S. Ramalingam, M. Naresh Babu, Y. Devarajan, M. Dinesh Babu, E.G. Varuvel, Environmental and energy valuation of waste-derived Cymbopogon Martinii Methyl Ester combined with multi-walled carbon (MWCNTs) additives in hydrogen-enriched dual fuel engine, International Journal of Hydrogen Energy 48 (2023) 39641–39657.

[11] T. Sathish, K. Muthukumar, A.K. Abdulwahab, M. Rajasimman, R. Saravanan, K. Balasankar, Enhanced waste cooking oil biodiesel with Al2O3 and MWCNT for CI engines, Fuel 333 (2023).

SB-OP04 RAPID DETECTION AND DIFFERENTIATION OF BUTYRIC *VS.* ω-3 FATTY ACID MOIETIES IN DAIRY FOODS BASED ON COSY NMR SPECTRA

Alin-Andrei Barna[1], Cristina Elena Stavarache[2,3], Aurelia Bratu[1], Mihaela Tociu[1], Mihaela-Liliana Mihalache[1], Nicoleta-Aurelia Chira[1*]

[1] National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnology, "C. Nenitescu" Department of Organic Chemistry, 1-7 Gh. Polizu Street, 011061 Bucharest, Romania

[2] National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnology, Advanced Polymer Materials Group, Bucharest, Romania.

[3] "Costin D. Nenitescu" Institute of Organic and Supramolecular Chemistry, 202B Spl. Independentei, 060023, Bucharest, Romania

Abstract: *We report here a rapid method allowing for the simultaneous detection and differentiation of the butyric and linolenic moieties in dairy products based on COSY NMR spectra.*

Key words: ^{1}H-NMR, COSY, butyric moiety, dairy products (TNR 10)

Introduction: Milk fat distinguishes from other fats by important amounts of butyric acid (C4:0) and only traces of ω-3 fatty acids (*e.g.* linolenic acid, C18:3) [1]. On the other hand, vegetable oils such as rapeseed, soybean, linseed, may contain large quantities of C18:3 [2]. In the ^{1}H-NMR spectrum, the distinctive resonances of both C4:0 and C18:3 appear overlapped; therefore, the two species cannot be differentiated through ^{1}H-NMR [3]. COSY (*CO*rrelation *S*pectroscop*Y*) is a relatively rapid (15 minutes) 2D NMR technique that identifies adjacent nuclei (^{1}H) coupled to each other through covalent bonds. Hence, COSY-NMR may prove useful for fast visual differentiation of the end chain methyl groups from C4:0 and C18:3.

Experimental: ^{1}H-NMR and 2D-COSY spectra were recorded on a Bruker Advance III HD 600 MHz spectrometer (Bruker, Rheinstetten, Germany), corresponding to the resonance frequency of 600.12 MHz for the ^{1}H nucleus, equipped with a direct detection four nuclei probe head and field gradients on the *z* axis.

Results and discussions: Figure 1 presents the 2D-COSY NMR plot of a soybean oil-tributyrin binary mixture (4% tributyrin). The end chain -CH_3 protons in C4:0 are correlated with the -CH_2- group in the β position from the ester group in triacylglycerols. This homonuclear coupling is detected by COSY, which shows a cross-peak spot between the signal for the methyl protons (resonance **A**) and the resonance of the β methylene group (resonance **D**). Conversely, the methyl protons

* Corresponding author: nicoleta.chira@upb.ro

in C18:3 (also resonance **A**) are adjacent to allylic protons (resonance **E**); hence, this correlation results in a distinctive cross-peak spot in the COSY plots. Consequently, the different connectivity of the methyl group in butyric *vs*. linolenic moieties results in two distinctive spots (showcased in green and red, respectively) in the COSY plots, allowing for their differentiation (Figure 1).

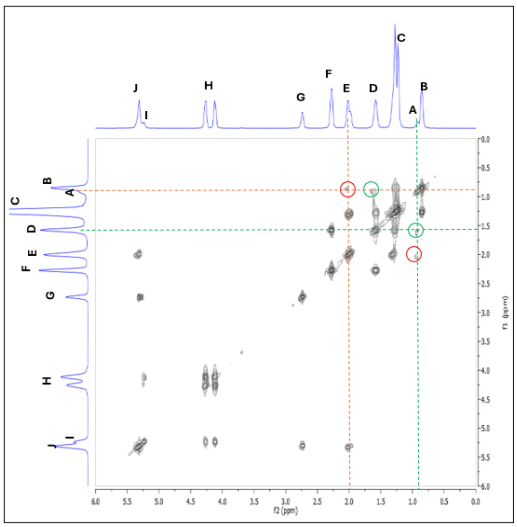


Fig. 1 COSY NMR spectrum of a soybean oil-tributyrin binary mixture (4% tributyrin).

Conclusions: Hence, COSY NMR technique can be useful for the rapid detection and differentiation of butyric and ω-3 fatty acids in a fat sample, thus revealing the addition of ω-3 containing oils of non-dairy origin into dairy foods within 20 minutes.

Acknowledgement:*This work was supported by a grant of the Ministry of Research, Innovation and Digitalization, CNCS-UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0756, within PNCDI IV.*

References:

[1] Bharwade M., Balakrishnan S., Chaudhary N., Jain A.K., Fatty Acid Profile and Physico Chemical Characteristics of Milk Lipids of Kankrej Cow, *Int. J. Curr. Microbiol. App. Sci.*, 6(8), (2017), 3035-3047.

[2] Dorni C., Sharma P., Saikia G., Longvah T., Fatty acid profile of edible oils and fats consumed in India, *Food Chem.*, 238, (2018), 9-15.

[3] Hanganu A., Chira N.A., When detection of dairy food fraud fails: An alternative approach through proton nuclear magnetic resonance spectroscopy, *J. Dairy Sci.*, 104(8), (2021), 8454-8466..

SB-OP05 RHEOLOGİCAL AND PRİNTABİLİTY EVALUATİON OF PEGDA HYDROGELS AT DİFFERENT CONCENTRATİONS FOR DLP PRİNTİNG

Ali Alparslan Celik [1,2], Melek Beyza Reyhanoglu [1,2*], Sumeyye Cesur [1,2], Oguzhan Gunduz [1,2]

[1] Center for Nanotechnology & Biomaterials Application and Research (NBUAM), Marmara University, Türkiye

[2] Department of Metallurgical and Materials Engineering, Faculty of Technology, Marmara University, Türkiye

Abstract: *Poly(ethylene glycol) diacrylate (PEGDA) has shown as one of the most versatile synthetic hydrogels in the area of biofabrication due to its tunable mechanical properties, biocompatibility, and rapid photopolymerization under mild conditions. Although its common use, achieving an optimal balance between viscosity, viscosity behavior, and print fidelity remains a major challenge for DLP Printing. Therefore, understanding the rheological and printability characteristics of PEGDA formulations at different concentrations is critical for ensuring structural fidelity and mechanical stability of printed samples.*

In this study, PEGDA hydrogels at 10% and 30% (w/v) concentrations were prepared and systematically investigated to evaluate their suitability for DLP 3D printing. Rheological characterization was performed using oscillatory shear rheometry to determine viscosity profiles, shear-thinning behavior, and viscoelastic response. Printability was evaluated using the Printability Index (Pr), which quantifies the geometric fidelity of printed square structures, and by direct observation of shape retention before and after UV curing at varying exposure times (5 and 20 seconds).

The 10% PEGDA formulation exhibited higher initial viscosity and clear shear-thinning behavior. The samples observed limited viscoelastic recovery after printed samples. At 5 seconds, the samples were unstable losing their intended square geometry and demonstrating minimal curing response. It is indicating inadequate crosslinking density. Conversely, the 30% PEGDA formulation presented intermediate viscosity and moderate shear-thinning behavior, which favored superior structural stability. The printed squares improved their shape more effectively after 20 seconds of UV curing, confirming enhanced crosslinking efficiency and higher crosslinking density.

Overall, increasing PEGDA concentration significantly improved printability and shape fidelity by enhancing viscosity, viscoelastic recovery, and crosslinking performance. These findings highlight the importance of optimizing PEGDA concentration to balance curing time, and mechanical integrity. This study provides valuable insights into the formulation–rheology–printability relationship of PEGDA hydrogels and supports their further development as customizable for advanced tissue engineering and regenerative medicine applications.

* Corresponding author: sumeyye.cesur@marmara.edu.tr

SB-OP06 ALGAL DIVERSITY AND BIOPOLYMER COMPLEXITY: STRUCTURAL ELUCIDATION OF EXOPOLYSACCHARIDES FROM MICROALGAE

Thomas Flahaut[1]*, Léa Gaume[1], Moussa Amroudine[1], Elodie Peghaire[1], Pascal Dubessay[1], Gwendoline Christophe[1], Alina-Violeta Ursu[1], Philippe Michaud[1], Guillaume Pierre[1,2]

[1]Clermont Auvergne INP, CNRS, Institut Pascal, Université Clermont Auvergne, F-63000 Clermont-Ferrand, France

[2]Institut Universitaire de France (IUF), 1 rue Descartes, F-75005 Paris, France

Abstract: *Partial structural elucidation of rhamnose-rich exopolysaccharides from microalgae and cyanobacteria*
Key words: Exopolysaccharides, microalgae, cyanobacteria, L-rhamnose, structural elucidation, biopolymers

Introduction: L-Rhamnose, a rare 6-deoxy sugar, has numerous applications in food, pharmaceutical, and cosmetic industries. Currently, its industrial production is mainly based on the hydrolysis of terrestrial plant biomass, a process that yields only limited quantities and requires arable land while generating substantial biowaste. Moreover, the resulting L-rhamnose is often contaminated with other monosaccharides and aglycone compounds, requiring multiple purification steps that rely on toxic, corrosive, or aromatic solvents [1]. Identifying alternative and sustainable sources of L-rhamnose is therefore crucial. The French Agence Nationale de la Recherche (ANR) RAh project [ANR-23-CE43-0011] aims to develop innovative strategies for the extraction and purification of L-rhamnose from underexplored biomass such as microalgae.

Experimental and/or Modelling: *Production of exopolysaccharides:* Exopolysaccharides (EPS) from seven microalgae (*Tetraselmis* RCC1564; *Diacronema* RCC3514, RCC3438, RCC4037; *Glossomastix* RCC3685, RCC3688 RCC3707) [2] and one cyanobacterium (*Synechococcales* specie) were produced under photoautotrophic batch culture in f/2 or BG11 media.; *Biochemical analysis:* The biochemical compositions of the EPS were determined using a combination of colorimetric assays and Fourier Transform Infrared (FTIR) spectroscopy. Monosaccharide distributions were assessed using a modified Kamerling method [3]. Further structural elucidation was achieved through methylation analysis, based on an adapted Hakomori protocol [4], which provides insights into glycosidic linkages and polysaccharides branching patterns.

* Corresponding author: Thomas.FLAHAUT@doctorant.uca.fr

Results and discussions: Monosaccharide profiling revealed a wide diversity of heteropolysaccharides structures among the eight EPS samples. Several strains produced rhamnose-rich EPS, notably *Tetraselmis* RCC1564, whose EPS contained approximately 66% (mol ratio) L-rhamnose, and *Diacronema* RCC4037, with 57% L-rhamnose. Glycosidic linkage analysis further highlighted the structural complexity and heterogeneity of these biopolymers. In addition, the occurrence of sulfate groups introduced another degree of variability in polymer architecture. Partial structural elucidation of the EPS was achieved, and a complete characterization strategy has been initiated for the EPS of *Glossomastix* RCC3688. This ongoing work includes Nuclear Magnetic Resonance (NMR) spectroscopy, which will clarify the sequence and structural features of monosaccharides within the polymer.

Conclusions: These findings provide a foundation for the targeted selection of Carbohydrate-Active enZymes (CAZy hydrolases and lyases) capable of depolymerizing these EPS to release L-rhamnose. Moreover, this study also enhances the understanding of microalgal exopolysaccharide structures, which is essential for establishing structure–function relationships in these biopolymers and advancing their biotechnological valorization.

References:

[1] Linhardt R.J., Bakhit R., Daniels L., Mayerl F., Pickenhagen W., Microbially produced rhamnolipid as a source of rhamnose, Biotechnology and Bioengineering, 33, (1989), 365–368.

[2] Gaignard C., Laroche C., Pierre G., Dubessay P., Delattre C., Gardarin C., Gourvil P., Probert I., Dubuffet A., Michaud P., Screening of marine microalgae: Investigation of new exopolysaccharide producers, *Algal Res.*, 44, (2019), 101711.

[3] Kamerling J.P., Gerwig G.J., Vliegenthart J.F., Clamp J.R., Characterization by gas-liquid chromatography-mass spectrometry and proton-magnetic-resonance spectroscopy of pertrimethylsilyl methyl glycosides obtained in the methanolysis of glycoproteins and glycopeptides, Biochem. J., 151, (1975), 491–495.

[4] Hakomori S.-I., A Rapid Permethylation of Glycolipid, and Polysaccharide Catalyzed by Methylsulfinyl Carbanion in Dimethyl Sulfoxide, J. Biochem., 55, (1964), 205–208.

SB-OP07 FROM DATA TO DISCOVERY: MACHINE-LEARNING-DRIVEN X-RAY DIFFRACTION ANALYSIS APPLIED TO PHASE-DIAGRAM CONSTRUCTION IN COMPLEX OXIDE SYSTEMS

Vasile-Adrian Surdu[1]*, Romuald Győrgy[2]

[1]Department of Materials Science, Faculty of Materials Science and Engineering, Transilvania University of Brașov, 29 Eroilor Blvd., 500036 Brașov, Romania

[2]Department of Chemical and Biochemical Engineering, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7 Gheorghe Polizu, 011061 Bucharest, Romania

Abstract: *The coupling of advanced data-science techniques with classical X-ray diffraction (XRD) methods is reshaping how we characterize crystalline materials and derive phase relations. In this work we bring together two complementary threads: (i) a review of machine-learning (ML) approaches applied to powder X-ray diffraction data [1], and (ii) a focused study of the pseudo-binary $BiFeO_3$–$EuFeO_3$ oxide system [2], where ML-aided XRD classification is used to assist in constructing the sub-solidus phase diagram. The review establishes the motivations for ML in XRD: increasing data volumes, overlapping diffraction peaks, noisy real-world measurements, and the need to speed up phase identification and quantification. It surveys supervised and unsupervised ML methods—such as cluster analysis, support-vector machines, deep neural networks—and addresses key limitations including dataset scarcity, interpretability, and robustness. The case study then applies a cluster-analysis algorithm to XRD patterns measured for $Bi_{1-x}Eu_xFeO_3$ ($x = 0 – 1$) compositions processed via solid-state reaction at various temperatures (800–1200°C). Eight distinct clusters were identified from the diffraction data, which helped guide subsequent traditional phase-identification and quantification by Rietveld (or related) refinement methods. The resulting phase diagram reveals six crystallization fields across the composition–temperature space, while underscoring the hybrid workflow: the ML step provides rapid classification, but the final diagram still required conventional analysis for accuracy. Together, these works illustrate a pathway towards high-throughput, ML-augmented XRD analysis and phase-diagram generation in complex materials systems. We conclude with a discussion of future trends: integrating constraints into ML models, real-time/operando XRD data streams, and closed-loop experimental workflows in materials discovery.*

Key words: X-ray diffraction, phase transitions, phase diagram, crystal structure, cluster analysis, machine learning, Rietveld refinement, $BiFeO_3$, $EuFeO_3$

References:

[1] Surdu V.-A., Győrgy R., X-ray Diffraction Data Analysis by Machine Learning Methods – A review, *Applied Sciences*, 13, 17, (2023), 9992.

[2] Surdu V.-A., Győrgy R., Phase Relations in the Pseudo-Binary $BiFeO_3$-$EuFeO_3$ System in the Subsolidus Region Derived from X-ray Diffraction Data – A Machine Learning Approach, *Inorganics*, 12, 12, (2024), 314.

* Corresponding author: vasile.surdu@unitbv.ro

BOOK OF ABSTRACTS

SICHEM – 2025

B – Applied organic, inorganic, and supramolecular chemistry in process engineering (AOISCPE)

3. Poster presentations

SB-P01 GAS DRYING BY ADSORPTION ON POROUS MATRIX COMPOSITE MATERIALS

Florin Bogdan[1], Mihai Albulescu[2*], Aurelian Șisinea[1]

[1]Ph.D. School, Petroleum-Gas University

[2]Oil and Gas Engineering Faculty, Petroleum-Gas University

Abstract: *A significant part of recent research in the field of gas adsorption is focused on obtaining adsorbent materials with improved adsorption capacity and achieving high heat and mass transfer rates. Extensive experimental studies on the physicochemical properties and several applications of composite materials used as adsorbents were carried out by Aristov, Liu and Wang and Zhang, respectively. All their studies showed that these adsorbents have a higher adsorption capacity than the classical ones and can be regenerated at a low temperature. Thus, for the purpose of drying gases by adsorption, composite materials obtained by impregnating porous host matrices with hygroscopic inorganic salts were used. Silica gel in the form of spherical granules and granules of arbitrary shape (angular), activated alumina granules and activated carbon granules were used as host matrices.*

Key words: gas drying, silicagel, matrix composites

Introduction: For the purpose of drying gases by adsorption, composite materials obtained by impregnating porous host matrices with hygroscopic inorganic salts were used [1].As host matrices, silica gel in the form of spherical granules and granules of arbitrary shape (angular), activated alumina granules and activated carbon granules were used. In the case of silica gel, the spherical granules had a diameter of 2.57 mm, and the angular ones, an average diameter of 2.25 mm. The activated alumina granules and activated carbon had average diameters of 0.15 mm and 0.1 mm, respectively [2].

In this way, four types of composite materials were obtained:

C – activated carbon,

M1 –composite material obtained by impregnating activated carbon with $CaCl_2$ (calcium chloride) solution - 15%;

M2- composite material obtained by impregnating silica gel (cornered granules) with CaCl2 (calcium chloride) solution - 15%;

M3 – composite material resulting from impregnating silica gel (spherical granules) with CaCl2 solution (calcium chloride) - 15%;

Experimental and/or Modelling: The values of temperature, vapor concentration in the gas phase and water concentration in the solid phase were experimentally determined at several values of duration (10, 30, 60, 90, 120, 150 minutes) and at different heights of the fixed adsorbent layer (0.08, 0.16, 0.24, 0.32 and 0.4 m),

* Corresponding author: malbulescu@upg-ploiesti.ro

Conclusion: The analyses showed that both the concentration of water vapor in the gas phase and the concentration of water in the adsorbent decrease over the height of the fixed bed. With increasing duration, the variation of the concentration C over the height is increasingly smaller. At high gas flow rates, in the upper part of the bed, this variation is insignificant, which highlights the existence of a saturated layer zone whose height continuously increases.
The concentration of water in the solid phase (X) also decreases over the height of the bed and with increasing duration and flow rate X increases. The temperature of the gas phase increases over the height of the fixed bed and presents a maximum at a certain value after which it decreases. At low values of duration, the maximum point is located at the upper part of the column and with increasing duration it moves towards the lower part of the fixed bed column.

References:

[1]. Dake, L.P., *Fundamentals of reservoir engineering*. Shell International Petroleum Maatschappij, Haga, 1978,
[2]. Lee, J., Wattenbarger R.A., *Gas Reservoir Engineering*, SPE Houston, Texas, 2004.

SB-P02 MOLECULARLY IMPRINTED FILMS FOR BIOMIMETIC SENSORS

Andrei Sarbu[1], Tanta Verona Iordache[1], Ana-Mihaela Gavrila[1], Anita- Laura Chiriac[1], Anamaria Zaharia[1], Teodor Sandu[1], Ana Lorena Neagu[1], Bianca Elena Stoica[1], Carmen Lazau[2]

[1]National Institute for Research & Development for Chemistry and Petrochemisatry - ICECHIM Bucharest

[2]National Institute for Research & Development for Electrochemistry and Condensed matter - INCEMC Timisoara

Abstract: *New molecularly imprinted film was obtained which can be used as sensitive layer for sensors*
Key words: Molecular imprinting, film, sensor

Introduction: Although considerable progress has been made in the last few decades, the field of chemo/biosensors remains underdeveloped and at a low commercialization level, due to the lack of alternative strategies and multidisciplinary methods. Therefore, research on chemo/biosensors based on a new detection concept has attracted wide interest in recent years. Molecular imprinting can generate recognition cavities in the cross-linked polymer network with the sterical and chemical information of the molecule used for imprinting, called template, which creates the premises for obtaining sensitive layers for sensors [1].

Experimental In order to obtain molecularly imprinted polymer films, the phase inversion method was preferred. The intention was to obtain films for explosive sensors, and therefore trinitrotoluene (TNT) was chosen as the template. Since the template used (TNT) is soluble in dimethylformamide, and this is a solvent used on an industrial scale, the synthesis of copolymers of acrylonitrile (AN) as a structural monomer with acrylic acid (AA) as a functional monomer (known for its ability to bind polar molecules) was preferred. Synthesis of acrylic copolymers was performed by the emulsion polymerization without emulsifier method.

Results and discussions : The molecularly imprinted polymer (MIP) films were comprehensively characterized by FTIR, thermal analysis, SEM and AFM, in comparison with non imprinted (NIP) film, to prove the success of the imprinting. For instance, in Figure 1 the FTIR characterization is presented

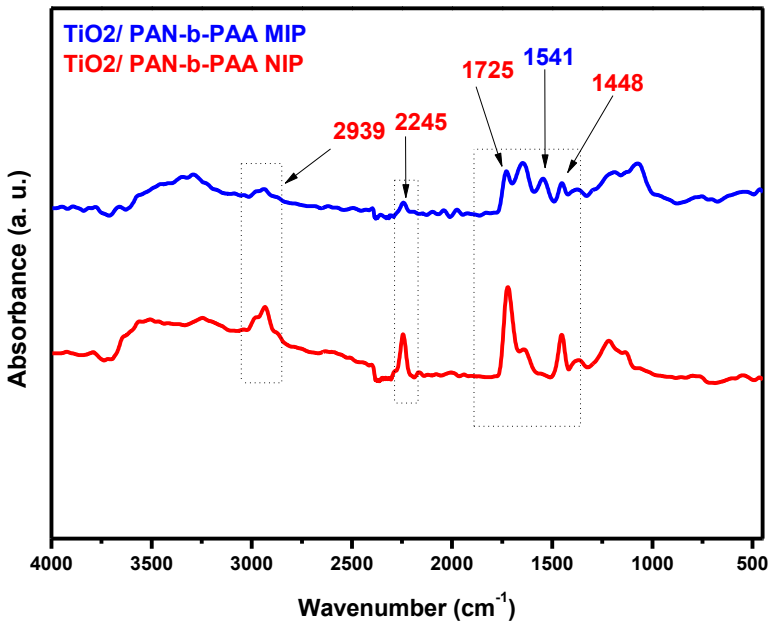


Fig. 1 FTIR Spectra of MIP and NIP films on FITO/TiO_2 support

Conclusions: Molecularly imprinted polymer films were produced with high recognition of trinitrotoluene target

Acknowledgments: This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CCCDI -UEFISCDI, project PN-IV-P2-2.1-TE-2023-1293 (ctr.40TE/2025) within PNCDI IV, and by an institutional grant of the Ministry of Research, Innovation and Digitalization, PN 23.06.01.01. AQUAMAT.

References:

[1] Carmen Lazau, Tanta-Verona Iordache, Ana-Mihaela Florea, Corina Orha, Cornelia Bandas, Anita-Laura Radu, Andrei Sarbu, Traian Rotariu "Towards developing an efficient sensitive element for trinitrotoluene detection: TiO_2 thin films functionalized with molecularly imprinted copolymer films" Applied Surface Science, 384, p. 449–458, 2016

SB-P03 MICROPOLUTANTS PRESENT IN DRINKING WATER

Georgeta Teodorescu (Diaconescu) [1*], Daniela Stefan [2*]

[1] University Politehnica Bucharest, Romania,

[2] University Politehnica Bucharest, Romania,

Abstract : *Micropollutants are a category of emerging contaminants that raise increasing concerns in the fields of environmental protection and public health, being detected in water sources at very low concentrations but with high toxic potential. These compounds originate from commonly used products such as pharmaceuticals, pesticides, personal care products, plastics, and industrial chemicals. Even after water treatment and purification processes, some of these pollutants persist and can reach drinking water, originating not only from environmental sources but also from materials used in water treatment and distribution infrastructure.*

The aim of this research was to evaluate the release of bisphenol A (BFA) from two types of plastic materials frequently used in the water sector: polystyrene (PS) and polyethylene terephthalate (PET). The study investigated how water physicochemical parameters, particularly pH and temperature, influence the amount of BFA transferred into the aqueous solution, as well as the structural changes undergone by the plastics after prolonged contact with water.

Experiments were conducted by exposing PS and PET samples to water at pH values ranging from 1.5 to 9, at two working temperatures (20°C and 30°C), over a period of 50 days. The concentrations of BFA released into the water were measured in ng/L, and structural changes in the materials were analyzed using infrared (IR) spectroscopy.

The results showed that polystyrene released higher amounts of BFA under acidic conditions, with maximum values of 4.72 ng/L at 20°C and 5.72 ng/L at 30°C at pH 1.5. As the pH increased, BFA concentrations decreased, indicating greater material stability in neutral and basic environments. Conversely, PET exhibited the opposite trend, with BFA release increasing with pH, reaching maximum values of 2.15 ng/L at 20°C and 2.87 ng/L at 30°C at pH 9, suggesting higher sensitivity in basic conditions.

IR spectra analysis confirmed structural modifications in PS, particularly at high pH, with variations in C=C and C–H vibration bands of aromatic and aliphatic chains, associated with substitution and partial degradation processes. PET showed a high degree of structural stability, with no significant changes in its characteristic ester functional groups (C=O, C–O).

In conclusion, the results highlight that plastic materials used in water treatment and distribution processes can act as secondary sources of organic micropollutants, especially under unfavorable pH and temperature conditions.

* Corresponding author: georgeta.teodorescu@upb.ro
* Corresponding author: simina_stefan-ro@upb.ro

Polystyrene appears more prone to BFA release in acidic media, while PET is more stable in neutral environments but more vulnerable in basic conditions. These findings emphasize the importance of selecting suitable materials for water treatment infrastructure to minimize the risk of drinking water contamination with toxic substances such as bisphenol A.

References:

[1] Bofill J. (2023) 'Microplastics and micropollutants in water', pp. 4–24.
[2] Gonsioroski, A., Mourikes, V.E. and Flaws, J.A. (2020) 'Endocrine disruptors in water and their effects on the reproductive system', International Journal of Molecular Sciences. MDPI AG, p. 21(6).
[3] Kim, M.K. and Zoh, K.D. (2016) 'Occurrence and removals of micropollutants in water environment', Environmental Engineering Research, 21(4), pp. 319–332.
[4] Loganathan, P. et al. (2023) 'Bisphenols in water: Occurrence, effects, and mitigation strategies', Chemosphere, 328, p. 138560.
[5] Priya, A.K. et al. (2022) 'Microplastics in the environment: Recent developments in characteristic, occurrence, identification and ecological risk', Chemosphere, 298.
[6] Sang, D. et al. (2022) 'Adsorption-desorption of organic micropollutants by powdered activated carbon and coagulant in drinking water treatment', Journal of Water Process Engineering, 49, p. 103190.
[7] Tao, H. et al. (2023) 'Variation of microplastics and biofilm community characteristics along the long-distance raw water pipeline', Process Safety and Environmental Protection, 169, pp. 304–312.

SB-P04 INVESTIGATING OF MASONRY ELEMENTS FOR SELECTING THE APPROPRIATE INORGANIC CONSOLIDANTS: THE CASE OF A ROMANIAN FUNCTIONAL BUILDING

Ludmila Motelica[1,2,4], Denisa Ficai[2,3,4], Ovidiu Cristian Oprea [2,3,4], Anton Ficai[1,2,3,4] , Roxana-Doina Trusca[4], Irina Fierascu[5,6], Radu Claudiu Fierascu[5] and Madalin Vasile Coman[7]

[1]Research Center for Advanced Materials, Products and Processes, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

[2]Academy of Romanian Scientist, Bucharest, Romania

[3]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania

[4]National Center for Micro and Nanomaterials, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

[5]National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM, 202 Spl. Independentei, 060021 Bucharest, Romania

[6]University of Agronomic Sciences and Veterinary Medicine of Buchaarest, 59 Marasti Blvd, 011464, Bucharest, Romania

[7]POP & ASOCIATII, Alea Barajului Cucuteni street, sector 3, Bucharest

Abstract: *The restoration technology of historical buildings currently finds itself in a period of transition between the old and the new, emerging technologies. The restoration work on stone objects or masonry requires a thorough understanding of the original materials, including their source, composition, and deterioration characteristics [1]. This is necessary to select appropriate, compatible, and durable replacement materials and repair techniques [2].*

Figure 1. Degraded brick masonry and plaster

The identification methods such as infrared spectroscopy (FTIR), ultraviolet and visible spectra (UV-Vis), photoluminescence spectra (PL), scanning electron microscopy (SEM) and FTIR microscopy were performed to show the distribution of individual chemical compounds that

constitute the building blocks. The use of modern research methods with a particular emphasis on the spectroscopic methods allowed for a thorough examination of the samples.

FTIR-ATR analysis of brick samples revealed the presence of vibrational bands specific to silicates, phyllosilicates, feldspars, carbonates and anhydrous clay minerals, indicating variations in mineralogical composition and firing temperature.

ACKNOWLEDGEMENT: The authors are acknowledging the support of the project: This work was supported by the Ministry of Education and Research (Ministry of Research, Innovation and Digitization), CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0522, 47PTE/2025 "Development of ecological solutions based on silanes and nanoparticles for the protection of buildings and monuments"-NanoConsol l and to the Romanian Government for providing access to the research infrastructure of the National Centre for Micro and Nanomaterials through the National Program titled "Installations and Strategic Objectives of National Interest"

The authors are grateful to the Romanian Government for providing access to the research infrastructure of the National Center for Micro and Nanomaterials through the National Program titled "Installations and Strategic Objectives of National Interest".

REFERENCE

[1] Fierascu R.C et al Jian M. et al Selected Aspects Regarding the Restoration/Conservation of Traditional Wood and Masonry Building Materials: A Short Overview of the Last Decade Findings *Appl. Sci.* **2020**, *10*(3), 1164; **https://doi.org/10.3390/app10031164**

[2] Toma Fistos et al Advancements in Stone Object Restoration Using Polymer-Inorganic Phosphate Composites for Cultural Heritage Preservation; Polymers 2024, 16(14), 2085; https://doi.org/10.3390/polym16142085

SB-P05 CORROSION INHIBITORS IN PETROLEUM PROCESSING

Andrei I. Chiriţă[1*], Ancaelena Eliza Sterpu[2], Olga Sapunaru[2], Tănase Dobre[1]

[1]National University of Science and Technology POLITEHNICA Bucharest, 1-7 Gheorghe Polizu Str., 011061 Bucharest, ROMANIA,

[2]Ovidius University Constanta, 124 Mamaia Boulevard, 900527 Constanța, ROMANIA

Abstract: *Corrosion remains a critical issue across the petroleum industry, affecting upstream, midstream and downstream assets. This paper reviews corrosion mechanisms and the use of inhibitors in refinery units, emphasizing the synergy between neutralizing and film-forming inhibitors. The study also introduces a CO_2 corrosion prediction model based on the De Waard–Milliams approach, adjusted for fugacity, pH, film formation, and inhibitor efficiency. A practical case involving a DN200 carbon steel valve (100 bar, 110 °C, pH 7, inhibitor 95%) is analyzed, yielding corrosion allowance values of 3 mm for 10 years and 6 mm for 20 years. The integrated approach links chemical inhibition, modelling, and materials selection to improve reliability in petroleum processing facilities.*

Key words*:* corrosion, inhibitors, De Waard-Milliams, film forming inhibitors, CO_2 corrosion

Introduction: Corrosion is one of the most significant degradation phenomena in the oil and gas industry, impacting on the mechanical integrity, safety, and economic performance of facilities across the entire petroleum value chain. According to the NACE International IMPACT study, global losses due to corrosion are estimated at over USD 2.5 trillion annually, representing 3–4% of the world's GDP [1]. Beyond the economic dimension, corrosion contributes to environmental risks and unplanned shutdowns that severely disrupt operations. In the petroleum industry, corrosion arises from the complex interaction of water, dissolved gases (CO_2, H_2S, O_2), acids (HCl, HF, H_2SO_4), and chlorides, often under high pressure and temperature. These aggressive agents attack metallic surfaces—particularly carbon steels—through electrochemical reactions that depend on pH, temperature, salinity, and flow regime. The problem manifests differently across production and refining systems: upstream, where high salinity and acid gases dominate, and downstream, where aqueous corrosion, acid dew points, and salt deposition prevail. To mitigate these effects, the industry employs a combination of material selection, design optimization, and chemical inhibition. Inhibitors are among the most effective and cost-efficient protection strategies, extending component life while allowing continued use of carbon steel. Two main categories are used: neutralizing inhibitors, which control condensate acidity, and film-forming inhibitors, which create hydrophobic protective barriers on metal surfaces [2].

Experimental: This study integrates the theoretical background of corrosion mechanisms with the practical use of inhibitors across refinery units and introduces a predictive CO_2 corrosion model based on the De Waard–Milliams (DWM) approach. The model, supported by experimental validation, enables accurate corrosion-rate estimation and

* Corresponding author: achirita998@gmail.com

corrosion allowance (CA) sizing, guiding safe and sustainable material selection in petroleum processing systems. The modelling analysis predicts CO_2-induced corrosion in a DN200 carbon steel under refinery conditions (100 bar, 110 °C, x_{CO_2} = 0.001 mol fr, pH = 7). A corrosion inhibitor with 95% efficiency without glycol injection was considered. The base rate was computed using the De Waard–Milliams method and corrected through process parameters such as CO_2 activity, pH, $FeCO_3$ film formation, and inhibitor efficiency, resulting in a realistic corrosion rate estimate.

Results and discussions: Carbon steel pipes and valves are widely used in **onshore applications** such as refineries and petrochemical plants. Their suitability for **CO_2-corrosive environments** must be justified by calculating the **corrosion allowance**.

The modelling study evaluates CO_2-induced corrosion in a device's components operating in a refinery conditions. The valve carries a corrosive oil stream at 100 bar and 110 °C, with a CO_2 molar fraction of 0.001 and pH = 7. No glycol injection was applied, while a corrosion inhibitor with 95% efficiency was introduced. The design life was analyzed for 10 years and respectively 20 years. The analysis confirms that the combined effect of $FeCO_3$ film stabilization and high inhibitor efficiency ensures long-term protection of carbon steel under refinery operating conditions.

Material Selection Criteria: If the **calculated corrosion allowance exceeds 3 mm**, the valve material should be replaced with a **corrosion-resistant material**, such as austenitic **stainless steel or duplex stainless steel.** A more common alternative is to use a **corrosion allowance of up to 6 mm** for carbon steels and low-alloy steels. **Corrosion-resistant alloys (CRA)** do **not require a corrosion allowance**, as they are inherently resistant to CO_2 corrosion. **Carbon steel is not commonly used offshore** due to external environment corrosion, corrosive species presence in pipes fluids flow, severe internal and external corrosion risks. If carbon steel valves are used offshore, their **resistance to CO_2 corrosion must be justified** using the proposed model or an alternative. Another approach is to **standardize the corrosion allowance** for carbon and low-alloy steels to **3 mm**, in accordance with **NORSOK M-001** standard for offshore use [3]. A corrosion allowance greater than 3 mm is **not recommended** for pipes and valves in the oil and gas industry, as it increases the **weight** of the components.

Conclusions: This study demonstrates that the integration of CO_2 corrosion modelling with the evaluation of inhibitor efficiency provides a reliable basis for predicting corrosion rates and selecting materials in petroleum processing systems. Using the De Waard–Milliams correlation and successive correction factors—fugacity, film formation, pH, aqueous phase, and inhibitor performance—the corrected corrosion rate for the investigated valve was reduced from 4.67 mm/year to 0.26 mm/year. For a 10-year design life, a 3 mm corrosion allowance (CA) is sufficient, while for 20 years, a 6 mm CA is required.

References: [1] NACE International IMPACT Report (2016), 15835 Park Ten Place, Houston, TX 77084; **[2]** L.T. Popoola, A.S. Gema, G. Latinwo, B. Gutti, A. Balogun, Corrosion problems during oil and gas production and its mitigation, Int. J. Ind. Chem. 4 (35) (2013); **[3]** Karan Sotoodeh,Chapter 4 - Carbon dioxide (CO2) corrosion, Editor(s): Karan Sotoodeh, Case Studies of Material Corrosion Prevention for Oil and Gas Valves, Gulf Professional Publishing, 2022, Pages 175-189

SB-P06 SPECTROSCOPIC INVESTIGATIONS ON THE DEGRADED PAINT OF HISTORICAL BUILDINGS

Ludmila Motelica[1,2,4], Denisa Ficai[1-4*], Anton Ficai [1-4], Roxana-Doina Trusca[4], Angela Spoiala[1,4], Ovidiu Cristian Oprea[2,4,5], Radu Claudiu Fierascu[2,3,5] and Irina Fierascu[5,6]

[1]Research Center for Advanced Materials, Products and Processes, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

[2]Academy of Romanian Scientist, Bucharest, Romania

[3]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania

[4]National Center for Micro and Nanomaterials, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

[5]National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM, 202 Spl. Independentei, 060021 Bucharest, Romania

[6]University of Agronomic Sciences and Veterinary Medicine of Buchaarest, 59 Marasti Blvd, 011464, Bucharest, Romania

Abstract: *Painted surfaces of the construction materials represents one of the most well-known challenges in the heritage science [1]. Throughout the ages, very different dyes and pigments were used to obtain visually similar colours. The visual appearance of these colours is also dependant on the substrate on which they are applied [2].*

Different types of coloured samples were collected from a heritage building in Cluj-Napoca (Romania), dating from aprox. 1900 and were thoroughly analysed and examined with analytical methods such as SEM, FTIR, PL and UV-Vis to evaluate their mineral composition, and microstructure. These investigations offer essential understanding for creating suitable restoration materials and maintaining the integrity of painted surface having historical relevance, considering the very complex, and long-term activity of the different physical, chemical and biological factors. A special attention in the restauration is to be paid to the painting surfaces, as these are more exposed and, also important, they are highly visible being the outer layer.

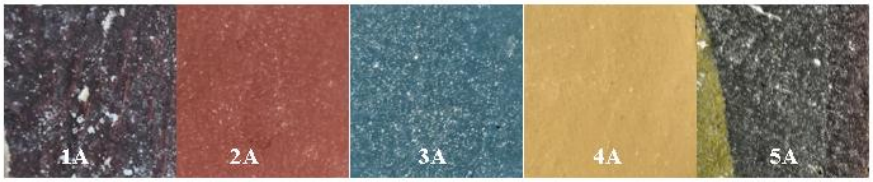


Figure 1. Optical appearance of the various painted samples from historical building

This investigation provides essential information for understanding the creation of appropriate restoration materials and maintaining the integrity of historical sites. Heritage is a legacy that we must participate in through a continuous process, being transmitted from one generation to the next, providing absolute value to the individuals and the community.

* Corresponding author: denisa.ficai@upb.ro

ACKNOWLEDGEMENT: The authors are acknowledging the support of the project: This work was supported by the Ministry of Education and Research (Ministry of Research, Innovation and Digitization), CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0522, 47PTE/2025 "Development of ecological solutions based on silanes and nanoparticles for the protection of buildings and monuments"-NanoConsol and to the Romanian Government for providing access to the research infrastructure of the National Centre for Micro and Nanomaterials through the National Program titled "Installations and Strategic Objectives of National Interest"

REFERENCE

[1]. Negri, A.; Nervo, M.; Di Marcello, S.; Castelli, D. Consolidation and Adhesion of Pictorial Layers on a Stone Substrate. The Study Case of the Virgin with the Child from Palazzo Madama, in Turin. *Coatings* **2021**, *11*, 624. https://doi.org/10.3390/coatings11060624

[2]. Aceto, M., Calà, E., Agostino, A., Fenoglio, G., Idone, A., Gulmini, M., & Picollo, M. (2017). Non-invasive study of the materials used in watercolour paintings by Gaudenzio Ferrari and his school. *Heritage*, **1**(1), 82–94. https://doi.org/10.3390/heritage1010007

SB-P07 A ROBUST TOP-DOWN METHOD FOR UNCERTAINTY ESTIMATION OF THE XRFS OUTCOMES CARRIED ON SOME UPCONVERSION FLUOROPHORES

Ion Pencea[1]*, Mihail Secu[2], Corina Secu[2], Elena Matei[2], Brindus Comanescu[3], Cristian Predescu[1], Andrei Berbecaru[1], Florentina Niculescu[1], Andrei L. Timis[1], George Coman[1]

[1] Faculty of Materials Science and Engineering, National University of Science and Technology Politehnica Bucharest (UNSTPB), 313 Splaiul Independentei, Romania

[2] National Institute of Materials Physics, Atomistilor 405A, 077125 Magurele, Romania

[3] OPTOELECTRONICA 2001, 35 Lake street, Măgurele, Romania, https://optoel.ro/

Abstract: *The paper substantiates a new robust top-down method for measurement uncertainty (MU) estimation of the ED-XRFS outcomes carried on up-conversion fluorophores (UCF). The SEM-EDS data were used to validate this top-down method. The entire philosophy of this paper subordinates to the following paradigm:* ***If you don't know the uncertainty of the measurement, don't make the measurement at all! [1]****.*

Key words: up-conversion fluorophores, measurement uncertainty, ED-XRFS, SEM-EDS

Introduction: The increasing demand for improving the product security has driven an increased interest towards the development of UCF taggants [2]. The ensuring a high quality of a spectral taggant imposes its exact composition measurement. XRFS is the most convenient for elemental analysis of UCP [3]. Thus, the validation of the XRFS results and adequate MU estimation is a must.

Experimental. The synthesis of the UCFs is fully described in a previous paper [3]. The measurements were carried with a SciAps X-200 spectrometer and a Zeiss Gemini 500 equipped with an EDS accessory from Bruker.

Results and discussions: The backgraunds of the top-down method for MU estimation, the characteristics of two sorts of UCFs, XRFS data processing and result validation through comparision among XRFS and SEM-EDS outcomes are posted in the paper. The top-down method we advanced is compliant with that given in Eurolab Technical Report 2007. The confidence intervals of XRFS results and of EDS ones ovelap in case both method measure the same element.

Conclusions: The method we advance is a novelty in the field of XRFS measurements carried on UCFs as it ensures a higher reliability of the results.

Acknowledgment. This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI-UEFISCCDI, project number PN-IV-P7-7.1-PTE-2024-0827, within PNCDI-IV.

References:

[1] *** *Calibration Uncertainty for Non-Mathematicians*, BEAMEX Calibration White Paper, available at www.beamex.com, accessed on October 22, 2025.; **[2]**. Senthamarai R., et.al., Recent advances in lanthanide-doped upconversion nanoparticles for optical anticounterfeiting, *Coordination Chemistry Reviews*, Elsevier, 542, (2025), 216892.; **[3]**. C. Bartha, C. E. Secu, E. Matei and M. Secu, Crystallization kinetics mechanism investigation of sol–gel-derived NaYF4:(Yb,Er) up-converting phosphors, *Cryst. Eng. Comm, 19 (*2017), 4992-5000, DOI: 10.1039/c7ce01265a;

* Corresponding author: ion.penecea@upb.ro; ini.pencea@gmail.com

SB-P08 DIFFERENTIATING OF RASPBERRY CULTIVATION REGIMES BASED ON ION CHROMATOGRAPHY CATIONS AND ANIONS PROFILING

Andreea Adelina Constantin[1,2], Geana Elisabeta-Irina[1,*], Corina Teodora Ciucure[1], Oana Romina Botoran[1], Roxana Elena-Ionete[1]

[1]National Research and Development Institute for Cryogenics and Isotopic Technologies, ICSI Rm. Valcea, Romania

[2]" Faculty of Agricultural Science, Food Industry and Environmental Protection, "Lucian Blaga" University of Sibiu, Romania

Introduction: Raspberry plants (*Rubus idaeus* L.) require precise nutrient management to optimize yield and fruit quality. Different cultivation regimes—such as agroforestry, organic vs. conventional fertilization, or varying fertilization levels—can influence the ionic composition of plant tissues, soil, or fruits [1]. Monitoring cation and anion profiles provides insights into plant nutritional status and can serve as a marker for cultivation practices. This study investigates the potential of ion chromatography (IC) to distinguish between agroforestry, organic and conventional raspberry cultivation systems, through detailed cation and anion profiling of raspberry fruits.

Experimental: Samples collected from different farming systems were analyzed for key cations (K^+, Ca^{2+}, Mg^{2+}, Na^+, NH_4^+) and anions (NO_3^-, NO_2^- PO_4^{3-}, SO_4^{2-}, Cl^-, F^-, Br^-) using high-performance IC. The study was conducted using two raspberry cultivars, Opal and Delniwa, harvested from two experimental organic plantations (organic in conversion (INMA Bucharest), and agroforestry system (Vladesti, Valcea) and compared with commercially sourced raspberry fruits from conventional production. Ripe raspberry fruits were harvested and frozen until analysis. The ionic profiles were analyzed using multivariate statistical methods, including principal component analysis (PCA) and hierarchical clustering analysis, to identify patterns linked to specific cultivation system.

Results and discussions: Among the analyzed cations, K^+ was the most abundant in raspberries, ranging from 1026–1472 µg/g in the conventional system and 696–2091 µg/g in the organic system. Ca^{2+} and Mg^{2+} varied between 64.8–131 µg/g and 74.2–174 µg/g, respectively, with higher levels in organic raspberries from INMA Bucharest. Na^+ was highest in organic raspberries from Vlădești agroforestry system. NH_4^+, an indicator of ammonium-based fertilizer use, ranged from 7.85–166.55 µg/g, with elevated levels in conventional raspberry fruits. Also, distinct anion signatures were observed, with SO_4^{2-} and PO_4^{3-} the dominant anions, with higher values in raspberry fruits from INMA Bucharest, ranging between 19.62-186.84 µg/g for SO_4^{2-} and from 14.10-255.27 µg/g for PO_4^{3-}. PCA analysis applied

* Corresponding author: irina.geana@icsi.ro

to the analytical data highlighted clear differentiation of the raspberry fruits based on the cultivation system. Raspberries from the Vlădești agroforestry system were distinctly separated from those cultivated under conventional and organic systems at INMA Bucharest (Figure 1). Additionally, within the INMA organic system, raspberries showed variety-specific separation (Delniwa – INMA-D and Opal – INMA-O), reflecting differences in ions uptake from the soil.

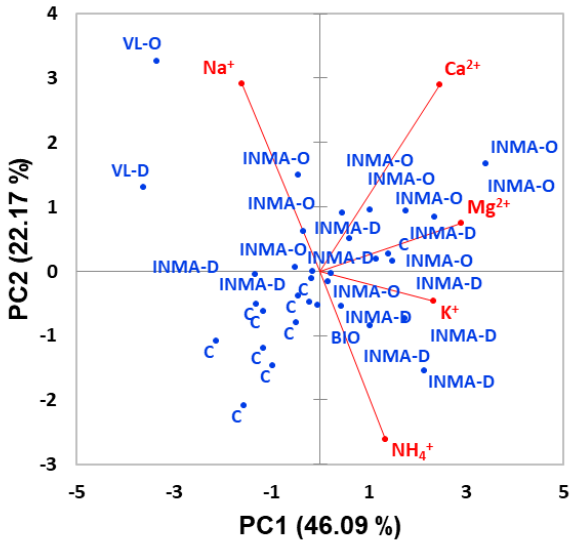


Figure 1. PCA analysis for differentiating raspberries according to cultivation system based on ions profiles

Conclusions: The results highlight that IC-based ion profiling can serve as a reliable, rapid, and precise approach for monitoring nutrient management practices, verifying cultivation methods, and supporting traceability in raspberry production. This methodology offers a practical tool for traceability, quality control, and the optimization of agronomic practices in berry farming.

Key words: raspberry fruits, cultivation system, ionic fingerprint, multivariate statistical analysis

Acknowledgments: This research was supported by project ***Establishment and operationalization of a Competence Center for Soil Health and Food Safety*** – CeSoH, Contract no.: 760005/2022, specific project no.5, with the title: *Improving soil conservation and resilience by boosting biodiversity and functional security of organic food products,* Code 2, financed through PNRR-III-C9-2022 – I5 (PNRR-National Recovery and Resilience Plan, C9 *Support for the private sector, research, development and innovation*, I5 *Establishment and operationalization of Competence Centers)* and PN 23150301, IsoProd.

References:

[1] G. Hasanaliyeva *et al.*, "Effect of Organic and Conventional Production Methods on Fruit Yield and Nutritional Quality Parameters in Three Traditional Cretan Grape Varieties: Results from a Farm Survey," *Foods*, vol. 10, no. 2, p. 476, Feb. 2021, doi: 10.3390/foods10020476.

SB-P09 SUSTAINABLE CHOLINE CHLORIDE/GLYCOLIC ACID-BASED NATURAL DEEP EUTECTIC SOLVENT FOR DUAL PLASTICIZING AND EXTRACTION IN CHITOSAN ACTIVE FILMS

Dragos Glavan[1], Paul Stanescu[1], Adina Gavrila[1], Gabriela Isopencu[1], Ludmila Motelica[2], Ovidiu Oprea[1], Adrian Nicoara[1], Sergiu Sima[1], Oana Ciocirlan[1,*]

[1]National University of Science and Technology Politehnica Bucharest, Faculty of Chemical Engineering and Biotechnologies, 132 Calea Grivitei, 010737, Bucharest, Romania

[2]National University of Science and Technology POLITEHNICA Bucharest, Advanced Research Center for Innovative Materials, Products and Processes, 313 Splaiul Independentei, 060042, Bucharest, Romania

Abstract: *We develop novel chitosan – natural deep eutectic solvent (NaDES) films with good mechanical and barrier properties, which can have good antimicrobial activity and antioxidant properties by incorporating plant extracts rich in polyphenolic compounds.*
Key words: Biodegradable, vegetal extracts, polyphenols, hawthorn, neem

Introduction: We explored choline chloride (ChCl)-glycolic acid (GA) NaDES as effective plasticizers for producing chitosan (CS) films. In addition, these NaDES systems were applied as extraction media for polyphenols from hawthorn (*Crataegus monogyna*) and neem (*Azadirachta indica*) leaves, enabling their direct incorporation into CS matrices. This dual functionality contributes to the development of bioactive films, a relatively new topic in the literature [1].

Experimental: Films were prepared by casting using ChCl-GA (1:3 molar ratio) NaDES, incorporating chitosan into formulations containing 44–70% NaDES. Plant extracts were obtained in aqueous solutions containing 30% NaDES.

Results and discussions: The incorporation of NaDESs and plant extracts into chitosan films resulted in notable performance improvements [2]. The films exhibited reduced Young's modulus values, confirming the plasticizing effect of the NaDESs. UV–Vis absorption analysis further showed that the presence of extracts broadened the absorption band from UVB into the UVA and visible regions, compared to extract-free films. FTIR spectra indicated strong molecular interactions, highlighting the formation of H-bonds between CS and NaDES, as well as between polyphenolic compounds and the polymer–NaDES network.

Conclusions: Films obtained with 50% NaDES were the most promising in terms of mechanical properties and water vapour permeability (WVP), which were improved by incorporating extracts.

References: **[1]** Zhao, Q., et al., Plasticization of gelatin/chitosan films with deep eutectic solvents and addition of *Flos Sophora Immaturus* extracts for high antioxidant and antimicrobial. *Food Hydrocol*. 160 (2025), 110752; **[2]** Jakubowska, E., et al. Physicochemical and storage properties of chitosan-based films plasticized with deep eutectic solvent. *Food Hydrocol*. 108 (2020) 106007

* Corresponding author: oana.ciocirlan@upb.ro

BOOK OF ABSTRACTS

SICHEM – 2025

C – Biomaterials and composites in chemical and biochemical applications (BCCBA)

1. Keynotes

SC-KN01 NANOCHEMISTRY-THE MOST REVOLUTIONARY BRANCH OF NANOTECHNOLOGIES

Viorica Mușat

"Dunărea de Jos" University of Galaţi

Centre of Nanostructures and Functional Materials-CNMF,

Laboratory of NanoChemistry - LNC

Abstract: *Starting from "All matter has a shape and all shapes matter" (G.A. Ozin and A.C. Arsenault, 2006),* ***nanoChemistry*** *today represents a "bottom-up" nanotechnology manufacturing that creates directly, by a dedicated chemical synthesis that allows controlling the size, shape, and surface properties, nanomaterials/nano-objects with targeted properties.*

Unlike chemistry that produces new substances with molecular properties related only to degrees of freedom of atoms in the periodic table, nanoChemistry introduced new degrees of freedom related to controlled modifications on nanometer-scale (up to 100nm) of structure, size and shape ("Size and shape dependent effects", L. Cademartiri, G. Ozin 2009 Concepts of Nanochemistry).

Nanochemistry is the most versatile nanotechnological approach, creating a wide variety of new composition, new structures, new shapes, reproducing or not those existing in nature, for emerging to new properties and advanced applications.

The presentation shows some results of research conducted by the Laboratory of NanoChemistry-CNMF-UDJG in collaboration with partners from CENIMAT-i3N Nova University of Lisbon, Fraunhofer IISB Institute of Erlangen, "I. G. Murgulescu" and "P. Poni" Institutes of the Romanian Academy, focusing on the synthesis of nanostructured materials for applications in transparent and flexible electronics, photocatalysis, antimicrobial and biomimetic coatings.

BOOK OF ABSTRACTS

SICHEM – 2025

C – Biomaterials and composites in chemical and biochemical applications (BCCBA)

2. Oral presentations

SC-OP01 ANTIMICROBIAL QUINOLONES ENCAPSULATED IN LIPOSOME

Lucia Pintilie[1]*,, Maria Maganu[2], Constantin Draghici[2], Miron Teodor Caproiu[2], Fawzia Sha'at[1], Ramona-Daniela Pavaloiu[1], Mădălina-Diana Gaboreanu[3], Ioana-Cristina Marinas[4]

[1]National Institute for Chemical-Pharmaceutical Research and Development 112 Vitan Av., Bucharest-3, Romania

[2]Institute of Organic and Supramolecular Chemistry „Costin D. Nenițescu" București ,

202B Splaiul Independentei, Bucharest 6, Romania

[3] University of Bucharest, Faculty of Biology, Department of Botany and Microbiology, 90 Panduri Street, Bucharest 5, Romania

[4] University of Bucharest, University of Bucharest Research Institute, Department of Life, Environmental and Earth Sciences, Bucharest, Romania, 90 Panduri Street, Bucharest 5, Romania

Abstract: *Antimicrobial resistance has increased in recent decades due to the extensive and indiscriminate use of antibiotics. The World Health Organization included antimicrobial resistance in the list of ten major threats to global public health in 2021. Six major bacterial pathogens, including third-generation cephalosporin-resistant Escherichia coli, methicillin-resistant Staphylococcus aureus, carbapenem-resistant Acinetobacter baumannii, Klebsiella pneumoniae, Streptococcus pneumoniae, and Pseudomonas aeruginosa, were found to have the highest resistance-related mortality rates in 2019. To answer this urgent call, the development of new pharmaceutical technologies and drug delivery systems seems to be the promising strategy against microbial resistance.The paper presents encapsulation studies of 4 quinolones (FPQ200, FPQ202, HPQ200 and HPQ202), obtained by chemical synthesis (by Gould-Jacobs method and characterized by physicochemical methods and biological activity. The liposomes loaded with quinolones were characterized by determining the entrapment efficiency, preparation yield and macroscopic analysis and the biological activity has been evaluated. The antimicrobial activity and inhibition of microbial adhesion of liposomal formulated synthetic compounds is strongly dependent on the chemical structure of the active principle. Among the tested formulations, FPQ202 stood out for its remarkable antimicrobial activity against Gram-positive (S. aureus, E. faecalis) and Gram-negative (K. pneumoniae, P. aeruginosa) bacteria, with evident bactericidal effects in kinetic and 24-h viability tests. In parallel, FPQ202 also demonstrated the highest efficiency in inhibiting microbial adhesion to an inert substrate, an essential aspect in preventing biofilm formation. Compound HPQ202 showed intermediate activity, while HPQ200 and FPQ200 had low efficiency or even potentially favorable effects on bacterial adhesion, especially in the case of Gram-positive strains. Regarding C. albicans, all formulations were shown to be antifungally ineffective, both in inhibiting growth and adhesion, suggesting an intrinsic resistance of the yeast under these experimental conditions. In conclusion, FPQ202 emerges as a promising candidate for the development of broad-spectrum antimicrobial agents with anti-biofilm capacity.*

Key words: quinolones; antimicrobial resistance, drug delivery system, liposomes, antimicrobial activity.

Acknowledgments: This work was carried out through the NUCLEU Program within the National Research Development and Innovation Plan 2022-2027, carried out with the support of MCID, project no. PN 23-28 01 01

* Corresponding author:

SC-OP02 EFFECT OF LASER SURFACE HEAT TREATMENT ON WEAR AND HARDNESS RESISTANCE OF METAL MATRIX COMPOSITE (AL 336.0 ALLOY- Y_2O_3)

Hussein Fawzi Hussein[1,*], Farqad Rasheed Saeed[1], Shaalan Bdaiwi Ahmed[1], Deleanu Iuliana Mihaela[2], Murad Majid Hussein[3]

[1] Scientific Research Commission, Baghdad, Iraq
[2] Chemical and Biochemical Engineering Department, Politehnica Bucharest Polizu Str. 1-7, 011061 Bucharest, Romania
[3] Computer Technologies Engineering, AL-Turath University, 10013 Al-Mansour, Iraq

***Abstract*:** *Laser surface treatment was applied to enhance the tribological properties of aluminum composite. The study involved varying weight percentages of Y_2O_3 (up to 10 wt%) in a 336.0 aluminum alloy, produced via stir casting. Composites were prepared by adding Y_2O_3 in weight ratios of 2%, 4%, 6%, 8%, and 10% to the aluminum alloy. The effects of laser surface treatment on wear resistance and hardness were examined. Dry sliding wear and micro hardness tests were conducted, and the treated surfaces were analyzed using optical microscopy. Results showed that laser-treated surfaces were free of voids and large cracks. Hardness increased due to the formation of a dense layer in the laser-treated region. Both wear resistance and hardness improved with higher reinforcement percentages, peaking at 6 wt% Y_2O_3 before declining. The treated surface layer exhibited superior tribological properties compared to the untreated surface.*
Key words: laser treatment, dry sliding wear, reinforcement

Introduction: Metal matrix composites are extensively used in industries due to their high strength-to-weight ratio, toughness, low density, and resistance to harsh environments such as corrosion and high temperatures. Recently, laser surface treatment of composite materials has gained attention as a high-functionality technique. By adjusting laser parameters, the physical and chemical behavior of the surface can be altered, resulting in a uniform surface. Laser treatment offers advantages over traditional methods, including faster processing, precision, cost-effectiveness, and localized treatment [1].

Material Preparation The aluminum alloy used in this study was sourced from discarded minibus pistons purchased locally. The Al-Mg alloy / Y_2O_3 composites were prepared by melting aluminum alloy with magnesium and varying amounts of Y_2O_3. Laser surface treatment was performed using a fiber laser with an average power of 30W, pulse duration of 120 seconds, frequency of 20 kHz, wavelength of 1064 nm, and a scan speed of 100 mm/s.

Results and Discussions: The addition of Y_2O_3 to the Al-Mg alloy matrix produced intermetallic compounds such as Al_3Y. The major phase was aluminum, with minor phases including Al_4MgY, $Al_2Y_4O_9$, Al_3Y, Al_3Mg_2, and $Al_8Si_6Mg_3Fe$.

As shown in figure 1, the microstructure of the laser-treated composites showed three distinct zones: the base metal, heat-affected zone (HAZ), and molten zone.

* Corresponding author: hussein.f.hussein@src.edu.iq

The molten zone exhibited a fine dendritic structure with uniform Y_2O_3 particle distribution. Agglomeration of Y_2O_3 particles between dendrites resulted in finer dendrite spacing.

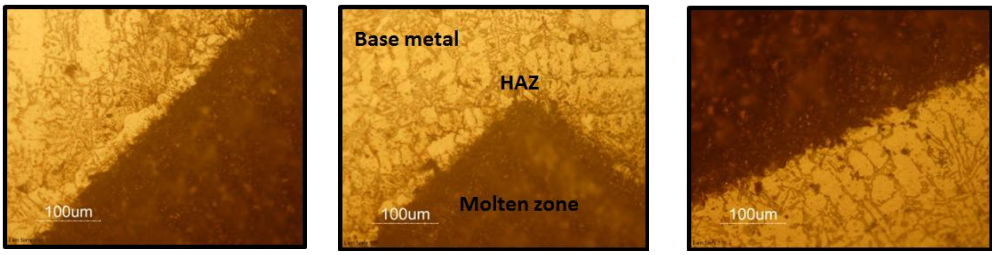


Fig. 1 The surface layer microstructure of composite after laser surface treatment: (a) Al-Mg alloy/ 2 wt% Y_2O_3 composite, (b) Al-Mg alloy/ 6 wt% Y_2O_3 composite, (c) Al-Mg alloy/ 10 wt% Y_2O_3 composite

The hardness of the Al-Mg / Y_2O_3 composites increased with the addition of Y_2O_3, peaking at 6 wt% before decreasing due to increased porosity. Laser treatment further enhanced hardness by improving bonding between reinforcement particles and the matrix. Laser-treated composites exhibited lower wear rates due to improved bonding and hardness.

Conclusions: Laser surface treatment proved to be an effective method for enhancing the hardness and wear resistance of aluminum matrix composites reinforced with Y_2O_3. The treatment not only improved the surface properties, but also minimized defects such as cracks and porosity, leading to better tribological performance. The optimal reinforcement level was found to be 6 wt% Y_2O_3, beyond which the benefits of reinforcement were offset by increased porosity. These findings suggest that laser surface treatment, combined with an appropriate reinforcement ratio, can significantly improve the mechanical and tribological properties of aluminum matrix composites, making them more suitable for industrial applications requiring high wear resistance and hardness.

References:

[1] Yilbas B. S., Karatas C., Karakoc H., Abdul Aleem B. J., Khan S., Al-Aqeeli N., Laser surface treatment of aluminum based composite mixed with B4C particles, Opt. Laser Technol., 65, 129-137, (2015).

SC-OP03 RECONFIGURING MEDICAL WASTE MANAGEMENT IN ROMANIA: CHALLENGES AND SOLUTIONS 2025

Adela Ciobanu*, Alexandru Ozunu[1]

[1] Faculty of Environmental Science and Engineering, University of Babeş-Bolyai, 30 Fantanele Street, RO-400294, Cluj-Napoca, Romania

***Abstract*:** *The transition from disposal to recovery and reuse of medical waste represents a strategic objective of the 2030 Agenda and of the circular economy in Romania. Adapting the Romanian legislative framework to the realities of 2025 should not be seen merely as a compliance obligation with European standards, but as a strategic opportunity to build an integrated medical waste management system that combines economic efficiency, health safety, and environmental protection. Romania currently applies regulations adopted in 2012 (Order of the Ministry of Health no. 1226), which no longer meet current requirements for public health protection, environmental safeguards, and integration into the European circular economy. The current legal framework, fragmented and often misaligned with the profile of waste generators, requires restructuring and modernization, with a clear differentiation between the requirements applicable to large healthcare facilities with complex and continuous waste flows, and those applicable to small-scale generators (individual medical practices or outpatient clinics), which produce smaller volumes but of the same hazardous nature.*

Modern medical waste treatment technologies, particularly thermal microwave sterilization integrating shredding and homogenization processes, demonstrate efficiency rates of over 90–99% in neutralizing pathogens and allow for volume reduction of up to 80–90%. These processes transform hazardous waste into inert fractions that can be reused as secondary resources in other industries, such as molecular disintegration, directly contributing to the objectives of the circular economy. At the same time, the digitalization of waste management flows through sensors, smart channels, and real-time traceability systems ensures efficient monitoring, strict risk control, and cost optimization.

This paper emphasizes the need to adapt national legislation to support the recovery of medical waste, including thermally treated waste, instead of a traditional approach focused exclusively on elimination through incineration. The new regulatory framework should promote the reintegration of the resulting materials into controlled productive cycles, transforming Romania's medical waste management into a field of innovation and sustainability. Such a shift would reduce pressure on landfills, improve sanitary safety, and bring economic benefits through the valorization of secondary resources. The paper presents recommendations derived from market research at the national level on medical waste traceability as of 2025.

In conclusion, at present there is no official document under public debate that provides a unified set of updated legislative norms for Romania regarding integrated medical waste management. However, various institutions and national authorities, such as the National Institute of Public Health, the National Environmental Protection Agency, and the Competition Council, have elaborated guidelines, reports, and plans addressing specific aspects of this field

Keywords:, incineration, sterilization, circular economy, pollution, alternative methods, competitive advantage, Medical waste treatment facilities

* Corresponding author: adela.romeghea@ubbcluj.ro

SC-OP04 EXTRACTION AND APPLICATION OF ALGAL CELLULOSE IN BIOPOLYMER PRODUCTION

Doinița-Roxana Tîrpan [1]*, Claudia Ana Maria Patrichi[2] and
Alina Georgiana Ciufu[2]

[1] Ovidius University of Constanta, Chemistry and Chemical Engineering Department, 124 Mamaia Blvd., 900527, Constanta, Romania

[2] University Politehnica of Bucharest, Chemical and Biochemical Engineering Department, 1-6 Gheorghe Polizu, 011061, Bucharest, Romania

Abstract: *In this sudy, membranes were obtained using cellulose extracted from algae.*
Key words: *Ulva lactuca*, cellulose, membrane, biopolymer

Introduction: In modern society, synthetic polymers are used in abundance in various fields due to their good mechanical properties and low price. However, the nondegradable behavior of polymers obtained from fossil fuels leads to environmental damage. Algae are a sustainable source for the global demand of biopolymers without affecting food supply. Biopolymers from algae seem to have great perspectives due to their high photosynthetic efficiency. Also, *Ulva lactuca* sp. has a high growing rate and can be found even in wastewaters or salt waters.
Experimental: In this study was implemented a procedure for extracting cellulose from *Ulva lactuca* sp. A physico-chemical characterization of the algal powder was made, but also of the biocellulose obtained from the algal material: optic microscopy, SEM and FTIR. The extraction of biocellulose was performed through ethanol precipitation which includes the removal of lipids, pigments, ulvans and hemicelluloses.
Results and discussions: The highest yield of extracted cellulose (20,944%) was obtained for the following factors: S/L=1/20; conc. ethanol=90%, conc. salts=4g/L this proving that *Ulva lactuca* is a viable alternative resource in cellulose production. Also, a procedure was performed to obtain membranes from cellulose extracted from the algal species. The swelling of biocellulose membranes in alcoholic solutions of high concentrations was investigated. It was observed that the process of absorption of the alcoholic solution by the membrane occurs rapidly in the first part. After stabilization, the membranes continue to absorb at a slower rate until saturation concentration is reached.
Conclusions: The purpose of studying and developing membranes is to use them in the processes of separation of alcohol-water mixtures for solvent recovery.
References:

1. Azeem M, Batool F., Iqbal N., Ikram-ul-Haq –Chapter 1 - Algal-Based Biopolymers, 2017, Chemistry, Biotechnology and Materials Science, pp. 1-31.

* Corresponding author: tirpanroxana@gmail.com

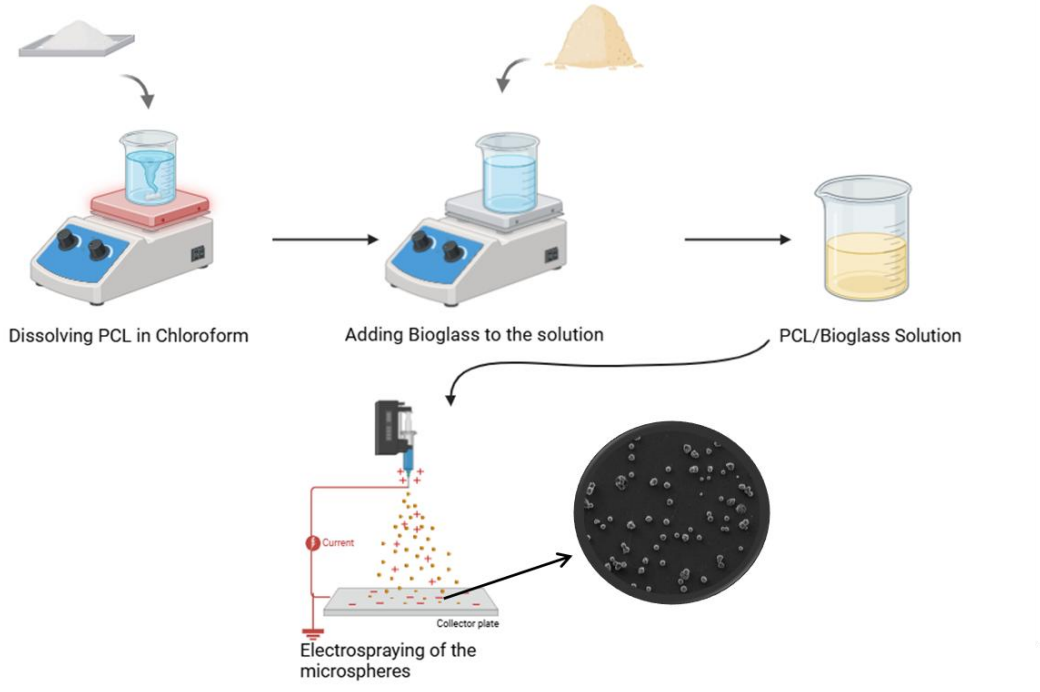
SC-OP05 FABRICATION AND CHARACTERIZATION OF PCL/BIOGLASS COMPOSITE MICROSPHERE COATINGS VIA ELECTROSPRAYING FOR ENHANCED SURFACE COMPATIBILITY IN BIOMATERIALS

Eray Altan[1], Şilan Tekin[1], Dilshat Tulyaganov[2], Oğuzhan Gündüz[1]

[1] Marmara University, Nanotechnology and Biomaterials Application and Research Center (NBUAM), Istanbul, Türkiye

[2] Turin Polytechnic University in Tashkent, Uzbekistan

Graphical Abstract



Abstract: *In this study, poly(ε-caprolactone) (PCL)/Bioglass composite microspheres were fabricated via the electrospraying method to improve the surface compatibility of biomaterials. The main objective was to develop a bioactive coating with enhanced cell interaction and potential use in tissue engineering applications. A 3% (w/v) PCL solution was prepared by dissolving PCL in 10 mL of chloroform and stirring at 250 rpm for 1 hour at room temperature. After obtaining a homogeneous PCL solution, Bioglass particles were incorporated at five different concentrations (0%, 2.5%, 5%, 7.5%, and 10% by weight) and stirred at 300 rpm for 1 hour to obtain homogeneous biocomposite solutions.In the electrospraying process, optimization of the flow rate, applied voltage, and tip-to-collector distance is crucial for obtaining well-defined particles. For the prepared biocomposite solutions, the experimental parameters were set as follows: an applied voltage of 12.5 kV, a flow rate of 0.5 mL/h, a tip-to-collector distance of 12.5 cm, and a spraying duration of 2–3 hours. These conditions were optimized to ensure stable jet formation and*

consistent particle morphology. The resulting coatings were characterized using Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and Differential Scanning Calorimetry (DSC). SEM analysis revealed well-distributed microspheres with controlled diameters and uniform morphology. FTIR and DSC analyses confirmed the successful incorporation of Bioglass within the PCL matrix without disrupting the polymer's crystalline structure. Moreover, cell viability assays demonstrated the biocompatibility of the coatings, showing no cytotoxic effects and supporting cell adhesion. In conclusion, electrosprayed PCL/Bioglass coatings exhibit promising characteristics as biocompatible surface layers for biomedical implants and tissue engineering scaffolds. The tunable composition and controlled morphology achieved in this work demonstrate the potential of this simple and effective fabrication approach for next-generation bioactive coatings.

SC-OP06 EUTECTOGELS BASED ON DEEP EUTECTIC SOLVENTS INCORPORATING METALLIC NANOPARTICLES FOR WOUND HEALING APPLICATIONS

Alexandra Ginga[1,2], Ionela Petcu [1,2], Teodora Tomescu[2], Oana Brincoveanu[1], Alexandra Mocanu[1], Andrada Serafim[2], George Vlasceanu[2], Roxana Cristina Popescu[2,3], Adela Banciu[2], Sabrina State (Rosoiu)[1, 2, *]

[1] National Institute for Research and Development in Microtehnologies, Ilfov, Romania

[2] National University of Science and Technology POLITEHNICA Bucharest, Romania

[3] "Horia Hulubei" Institute for Physics and Nuclear Engineering, Magurele, Romania

Abstract: *Alginic eutectogels were prepared using deep eutectic solvents (DES) based on choline chloride (ChCl) mixed with one of three hydrogen bond donors (HBD) – propanediol (PG), ethanediol (EG), glycerol (Gly) – to obtain stable, biocompatible matrices. Gold and silver nanoparticles (AuNPs, AgNPs) were then formed using alginate as gelling and reducing agent and polyvinylpyrrolidone (PVP) as stabilizer. PG-gels showed the best biocompatibility, while AgNPs provided antibacterial activity, supporting their potential for advanced wound healing applications.*

Key words: *deep eutectic solvents; eutectogels; silver nanoparticles; gold nanoparticles*

Introduction: Chronic wounds are difficult to treat and conventional hydrogels dry fast. Eutectogels, a new class of DES-based materials (first reported in 2018), provide stronger hydrogen bonding and stability. AuNPs and AgNPs show antimicrobial, anti-inflammatory, and regenerative effects, improving healing when integrated into these matrices. This work reports alginic eutectogels with *in situ* generated AuNPs and AgNPs, for wound healing applications [1,2].

Experimental: *Reagents:* Choline chloride, glycerol, ethanediol, propanediol, sodium alginate (SA), $HAuCl_4$, $AgNO_3$, PVP; *Preparation of eutectogels:* The three studied ChCl-based DES (ChCl:Gly, ChCl:PG, ChCl:EG) were mixed with SA to form gels. *Synthesis of NPs:* AuNPs and AgNPs were generated *in situ* using $HAuCl_4$ and $AgNO_3$ respectively as precursors, with SA as both gelling and reducing agent and PVP as stabilizer.

Results and discussion : Gelation depended on HBD type: Gly 20%, EG 40%, PG 70%. Rheology ($G' > G''$) confirmed gel behavior. Fourier Transformed Infrared Spectroscopy (FTIR) showed stronger O–H interactions, suggesting a hydrogen-linked network. PG-gels were biocompatible, while EG and Gly-based gels were more cytotoxic. UV-Vis spectroscopy results showed dispersed AuNPs (~530 nm) and partially aggregated AgNPs (~420 nm), both stabilized by PVP as reflected in the slightly blue-shifted bands. Antibacterial assays showed that AgNP-based eutectogels inhibited bacterial growth across all studied strains.

Conclusions: Alginic eutectogels with *in situ* AuNPs and AgNPs were obtained. PG-based systems showed best biocompatibility and antimicrobial potential.

* Corresponding author: sabrina.state@imt.ro, sabrina.rosoiu@upb.ro

Acknowledgements: The presented work was supported by several scientific national projects: The Romanian National Grant GNAC ARUT 2023 project (No. 7/06.10.2023), NANO_NP_DES, Core project number PN 2307 8N/03.01.2023, μNanoEl, within PNCDI IV (2022-2027), The Ministry of Education and Research, CCCDI - UEFISCDI, project number: PN-IV-P7-7.1-PTE-2024-0305, contract 40PTE/2025.

References:

[1] Liu Y., et al., *Natural Deep Eutectic Solvents: Properties, Applications, and Perspectives*, J. Nat. Prod., 81(3), (2018), 679–690.

[2] Mercadal P. A., Carretero-González J., Shapira E., Cuadrado C., *Eutectogels: The Multifaceted Soft Ionic Materials of Tomorrow*, JACS Au, 4, 10, (2024), 3744–3758.

SC-OP07 DEVELOPMENT AND CHARACTERIZATION OF HYDROXYAPATITE-REINFORCED SILKMA COMPOSITE SCAFFOLDS FABRICATED VIA DLP 3D PRINTING FOR BONE TISSUE ENGINEERING

Dilruba Baykara[1],Mine Akca[1],Oguzhan Gunduz[1]

[1] Marmara University, Nanotechnology and Biomaterials Application and Research Center (NBUAM), Istanbul, Türkiye

Abstract: *The treatment of bone defects remains a significant challenge in clinical practice. Bone tissue engineering (BTE) has emerged as a promising alternative to conventional treatment methods, aiming to promote bone regeneration by providing temporary mechanical and biological support through three-dimensional (3D) porous scaffolds.*

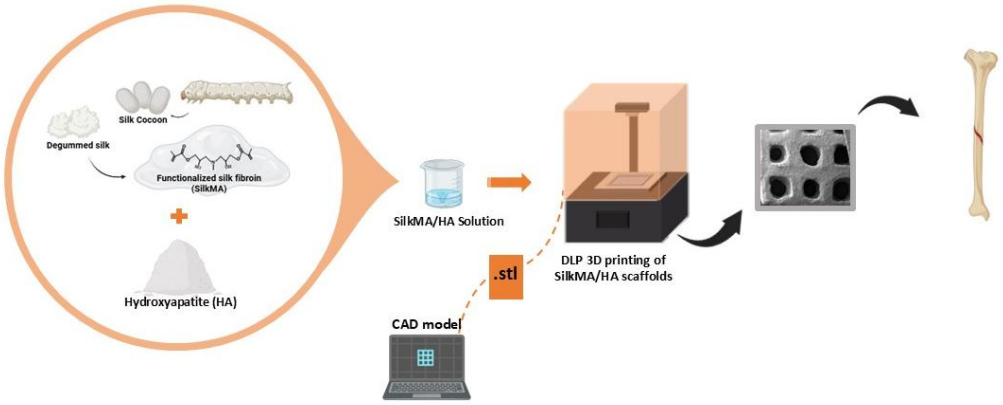
In this study, methacrylated silk fibroin (SilkMA) and hydroxyapatite (HA) composite scaffolds were fabricated via Digital Light Processing (DLP) 3D printing for potential application in bone defect repair. Following a biomimetic approach, SilkMA solutions (% w/v) containing 10% or 20% w/v HA were prepared at room temperature and stirred at 100 rpm for 30 minutes. A photoinitiator, lithium phenyl-2,4,6-trimethylbenzoylphosphinate (LAP), was added at a concentration of 0.25% (w/v) and mixed for an additional 10 minutes. Scaffold models were designed using SolidWorks 2020 (Dassault Systèmes SE, France) and printed with a Phrozen SonicMini 8K printer (Phrozen Tech Co., Ltd., Taiwan) operating at a wavelength of 405 nm, a light intensity of 12 mW/cm², and an exposure time of 30 seconds. The resulting SilkMA, SilkMA/10HA, and SilkMA/20HA scaffolds were successfully fabricated and systematically characterized in terms of their morphological, physical, and mechanical properties.

Characterization results obtained from scanning electron microscopy (SEM), swelling tests, and compression testing revealed that the incorporation of HA significantly influenced the morphology, mechanical performance, and hydrophilic behavior of the scaffolds. In particular, compression test results demonstrated that the HA-reinforced composites exhibited substantially higher compressive strength and stiffness compared to the pure SilkMA scaffolds, indicating that HA reinforcement effectively improved the overall mechanical integrity. SEM analysis confirmed that the scaffolds possessed a highly interconnected, uniform, and well-defined porous architecture, highlighting the superior resolution and precision of the DLP fabrication technique. This controlled microarchitecture is expected to facilitate efficient cell adhesion, proliferation, and nutrient transport. Additionally, swelling analysis demonstrated that the scaffolds exhibited a controlled water absorption capacity, maintaining a moist microenvironment suitable for cell survival and tissue regeneration without excessive swelling.

In conclusion, the synergistic combination of enhanced mechanical strength, optimized pore architecture, and favorable swelling behavior makes the DLP-printed SilkMA–HA composite scaffolds highly promising biomaterials for bone regeneration applications.

Keywords: Methacrylated Silk Fibroin, hydroxyapatite, DLP 3D printing, Bone tissue engineering

Graphical Abstract



SC-OP08 MODIFICATION OF BACTERIAL CELLULOSE FOR WOUND DRESSINGS USING SILVER NANOPARTICLES AND PROPOLIS EXTRACTS

Gabriela Isopencu[1], Edina Rusen[1], Gabriela Toader[2], Aurel Diacon[2], Sabrina State (Rosoiu)[3,4], Oana Brincoveanu[4], Cosmin Romanițan[4], Kliment Zanov[5], George-Mădălin Dănilă[5], Alexandra Mocanu [1,4,*]

[1] NUST POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, Dept of Chemical and Biochemical Engineering, 1-7 Gh. Polizu, 011061, Bucharest, Romania

[2]Military Technical Academy "Ferdinand I", 39-49 George Coșbuc Boulevard, 050141 Bucharest, Romania,

[3]NUST POLITEHNICA Bucharest, Faculty of Medical Engineering, 1-7 Gh. Polizu, 011061, Bucharest, Romania

[4] National Institute for Research and Development in Microtehnologies, 126A Erou Iancu Nicolae, 077190, Voluntari, Ilfov, Romania

[5]CROMATEC PLUS S.R.L., 1 Petre Ispirescu Street, 077167, Tâncăbești, Ilfov, Romania

Abstract: *This study investigates the development of wound dressings based on natural polymers like bacterial cellulose (BC) in the form of medical patches modified with silver nanoparticles (AgNPs), and hydroalcoholic propolis extracts. The pristine BC, BC modified with Ag and propolis extracts were investigated by scanning electronic microscopy (SEM) coupled with energy dispersive system (EDS), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and antimicrobial testing. The study demonstrated the selective synergistic effect of AgNPs and propolis extracts and medium antimicrobial efficacy against Escherichia coli (E. coli), Bacillus subtilis (B. subtilis), and Candida albicans (C. albicans) pathogen microorganisms.*

Introduction: Bacterial cellulose (BC) is a natural polymer synthesized extracellularly by non-pathogenic aerobic bacteria, such as *Komagataeibacter xylinum*, when grown in a culture medium containing carbon and nitrogen sources [1], native BC lacks inherent antimicrobial activity. Therefore, many studies have aimed to modify BC's properties to create antimicrobial BC-based dressings with improved tissue regeneration potential. Thus, the main aim of this work is to modify BC with *in situ* generated silver nanoparticle (AuNPs). Building on previous studies [2], it has been anticipated a synergistic effect between hydroalcoholic propolis extracts and (AgNP)-modified bacterial cellulose (BC) against pathogen microorganisms like *E. coli*, *B. subtilis.*, and *C. albicans*.

Experimental: *Synthesis of BC:* BC was produced using a modified version of the classic Hestrin–Schramm culture medium containing 2% (w/w) carbon source. The medium consisted of pulp-free berry juice supplemented with peptone and mineral salts and was incubated under static batch conditions at 28 °C for 7 days [1]. Prior

* Corresponding author: alexandra.mocanu@imt.ro

to use, BC was purified in NaOH solution (5% wt.) and washed several times afterwards with demineralized water until neutral pH. *In situ synthesis of AgNPs:* AgNPs were generated *in situ* in the presence of BC *(2 x 2 cm^2)* using $AgNO_3$ as precursor, and $Na_3C_6H_5O_7$ as reducing agent. *Impregnation with propolis extracts:* BC-Ag nanocomposites were impregnated with different hydroalcoholic propolis extracts [3].

Results and discussion: BC and modified BC was analyzed by SEM, FT-IR and XRD which indicated the purity of BC on one hand, and the AgNPs modification on the other. The presence of hydroalcoholic propolis extracts was evidenced by SEM. The pristine BC, BC-Ag, respectively BC-Ag-propolis composites were evaluated for antimicrobial synergistic effects against *E.coli, B. subtilis* and *C. albicans*.

Conclusions: The synergistic effect was registered depending on the propolis extract indicating selective medium antimicrobial activity against *C. albicans* at higher water content, respectively against *E. coli* at higher alcoholic content of the propolis extract.

Acknowledgements: This work was supported by The Ministry of Education and Research, CCCDI - UEFISCDI, project number: PN-IV-P7-7.1-PTE-2024-0305, contract 40PTE/2025, Core project number PN 2307 8N/03.01.2023, μNanoEl, within PNCDI IV (2022-2027), and the Romanian National Grant GNAC ARUT 2023 project (No. 7/06.10.2023), NANO_NP_DES.

References:

[1] G.O. Isopencu, A Stoica-Guzun, C. Busuioc *et.al*., *Development of antioxidant and antimicrobial edible coatings incorporating bacterial cellulose, pectin, and blackberry pomace*. *Carbohydrate Polymer Technologies and Applications* 2021, *2*, 100057.

[2] A. Mocanu, A.; G. Isopencu, G.; C Busuioc et. al., *Bacterial cellulose films with ZnO nanoparticles and propolis extracts: Synergistic antimicrobial effect*. Sci. Rep. 2019, 9 (1), 17687.

[3]. A. K. Saleh, J. S Albrahim, H. Alenezi, *Ex situ functionalization of bacterial cellulose with ethanolic extraction of propolis for enhanced antimicrobial performance*. Biomass Conversion and Biorefinery, 2025, 15(8), 12995-13010.

SC-OP09 ACETYLSALICYLIC ACID–VITAMIN K LOADED PCL STENTS FABRICATED BY FDM 3D PRINTINGS AS A POTENTIAL VASCULAR IMPLANT MATERIAL

Şevval Güneş[1], İsmail Ateş[1], Şimal Çeltikci[1], Ömer Faruk Saraç[1], Oğuzhan Gündüz[1], Canan Doğan[1], Ayşe Ceren Çalıkoğlu Koyuncu [1]

[1] Marmara University, Nanotechnology and Biomaterials Application and Research Center (NBUAM), Istanbul, Türkiye

Cardiovascular diseases (CVDs) remain the primary cause of mortality worldwide, creating a persistent need for safer and more effective vascular interventions. Conventional metallic stents, though efficient in restoring arterial patency, present long-term complications such as chronic inflammation, late thrombosis, and restenosis due to their permanent structure. This research focuses on developing a novel biodegradable, drug-eluting stent prototype capable of providing temporary mechanical support and controlled drug release.

The proposed stent is fabricated using polycaprolactone (PCL), a biocompatible and bioresorbable polymer known for its flexibility, stability, and non-toxic degradation profile. The design integrates a dual drug system composed of acetylsalicylic acid (ASA) and vitamin K, selected to achieve a balanced antithrombotic response. ASA acts as an antiplatelet agent to minimize thrombosis risk, while vitamin K regulates coagulation to prevent excessive bleeding—together promoting localized, safe hemostatic balance.

The stents were produced through fused deposition modeling (FDM)-based 3D printing, allowing precise control over geometry, porosity, and drug distribution. This method provides structural uniformity and facilitates customized scaffold fabrication aligned with physiological requirements.

Characterization analyses, including FTIR, DSC, SEM, mechanical testing, and MTT cell viability, were conducted to evaluate chemical, thermal, mechanical, and biological properties. The results indicated successful drug incorporation into the polymer matrix, mechanical stability compatible with vascular applications, and high biocompatibility with endothelial cells. Additionally, in vitro degradation and drug release studies demonstrated a sustained release pattern, suggesting the feasibility of controlled local therapy.

Overall, this study demonstrates the potential of 3D-printed PCL-based stents as an innovative alternative to permanent metallic implants. The combination of biodegradability, dual drug loading, and precise additive manufacturing introduces a promising approach to next-generation vascular scaffolds.

SC-OP10 CONDUCTIVE NANOCOMPOSITE HYDROGELS FOR NEURAL TISSUE ENGINEERING: A SYSTEMATIC SCOPING REVIEW OF RECENT TRENDS

Mohammad Moghaddasi[1], Busra Oktay[1], Ayse Betul Bingol[1], Reyhan Yanikoglu[1], Meryem Muslu[2], Ibrahim Tarik Ozbolat[3], Cem Bulent Ustundag*[1]

[1] Department of Bioengineering Yildiz Technical University Istanbul 34722, Turkey

[2] Department of Chemical Engineering Yildiz Technical University Istanbul 34210, Turkey

[3] Engineering Science and Mechanics Department Penn State University, University Park

Abstract: *Conductive nanocomposite hydrogels (CNHs) represent a versatile strategy in neural tissue engineering (NTE). This scoping review of 125 studies summarizes recent progress in CNH design, function, and therapeutic outcomes for both central and peripheral nervous system repair. For CNS applications, spinal cord injury (n = 42) is a major focus, with antioxidant–conductive and immunomodulatory hybrids used to reduce oxidative stress and neuroinflammation. In the PNS, notably sciatic nerve regeneration (n = 20), research emphasizes stimuli-responsive approaches (wireless, self-powered piezoelectric and magnetic systems) and biomimetic scaffold design which guide axonal growth. CNHs are also being explored for traumatic brain injury, stroke, Parkinson's disease, neurovascular niche reconstruction (e.g., diabetic wound healing), coordinated neurogenic/osteogenic repair, and cochlear neurogenesis. Overall, the field is shifting toward multifunctional, hybrid CNHs that combine electrical conductivity with biochemical and mechanical cues for targeted neural repair.*

Keywords: conductive hydrogel, nanocomposite, nanomaterial, neural differentiation

Introduction: Nervous tissue controls various processes such as sensation, movement, and cognition, but is vulnerable to trauma and neurodegeneration. CNS repair is constrained by inhibitory factors like glial scarring and relatively slower regenerative capacity mediated by Schwann cells in the PNS. [1] Hydrogels offer biocompatibility, high water content, tunable mechanics, and 3D-printing compatibility, but lack conductivity and often have limited bioactivity. Embedding conductive nanomaterials into hydrogels (forming CNHs) restores electrical pathways, strengthens mechanics, introduces nanotopography, and enables controlled release and electrical stimulation to better mimic the neural extracellular environment. [2] CNHs incorporate diverse conductive fillers such as carbon-based materials (CNTs, graphene derivatives, quantum dots), metal nanoparticles and SPIONs, conducting polymers (PANI, PPy, PEDOT), piezoelectric ceramics (e.g., $BaTiO_3$), and emerging 2D/semiconductor materials (MXenes, black phosphorus), each with its own unique properties. Mechanistically, CNHs recreate electroactive microenvironments that modulate membrane potential, open voltage-gated channels (driving Ca^{2+} signaling), and potentiate exogenous electrical stimulation via pathways like PI3K/Akt and MAPK/ERK. [3,4] Nanotopography and aligned structures provide contact guidance and mechanotransductive cues (e.g., PIEZO2, YAP/TAZ), while tuned stiffness and viscoelasticity permit cellular remodeling and neurite extension. [5] Surface functionalization and stimulus-responsive

* Corresponding author:

elements further enable targeted guidance, release, and scaffold reconfiguration, making CNHs versatile platforms for neural regeneration.

Methods and Study Selection: This scoping review followed PRISMA-ScR guidelines [6], and a protocol was pre-registered on the Open Science Framework on 26 September 2024. We searched PubMed (MEDLINE), Scopus, Web of Science, ScienceDirect, and Wiley for literature published mainly between 1 January 2020 and 31 December 2024, using tailored search terms (see Supplementary Files). Results were imported into Rayyan [7] for deduplication and screening, leaving 923 records. Title/abstract screening removed 685 records; full-text screening excluded a further 113, yielding 125 included studies. Eligibility prioritized studies that incorporated conductive nanostructures (0D–2D) and involved human or animal cells aimed at forming neural tissues or models. Neural-differentiation studies required clear induction methods and outcome measures (e.g., gene/protein analysis, morphology). Exclusions: studies without conductive nanostructures or cellular components, work unrelated to neural differentiation, non-English papers, non-original formats (reviews, opinions), inaccessible PDFs, or publications outside the 2020–early-2025 window. Data from the final 125 studies were extracted by blinded reviewers into MS Excel, cleaned and analyzed with Python (pandas), R (tidyverse), or Excel, and visualized with ggplot2.

Results: This review covers 125 studies published between 2020 and early 2025 on CNHs for NTE. Most studies focus on CNS repair—particularly spinal cord injury (n = 42)—followed by PNS targets such as the sciatic nerve (n = 20) and other specialized tissues like bone, epithelium, and cochlea. Neural differentiation (n = 28) also emerged as a key research theme. Commonly used cells included rodent-derived neural stem cells (NSCs, n = 40), mesenchymal stem cells (MSCs, n = 18), and PC12 cell lines (n = 28). Carbon-based nanomaterials dominated (36.8%), led by CNTs, GO, and rGO, followed by metals (24%) such as iron oxides and gold, and conductive polymers (16%) like PEDOT and PPy. Emerging semiconductors, ceramics, and hybrid magnetoelectric systems were also explored for multifunctionality. Natural polymers formed the majority of hydrogel backbones (61.4%), particularly polysaccharides such as gelatin, chitosan, alginate, and HA, while blended natural–synthetic systems addressed biocompatibility and mechanical challenges. Summary of select studies is as follows:

Li et al.'s wireless, ultrasound-activated piezoelectric hydrogel for spinal cord injury (SCI) integrates $BaTiO_3$-facilitated piezoelectricity and conductive PPy with localized Perampanel release to provide a non-invasive, on-demand electrical stimulation modality that mitigates inflammation and promotes motor recovery [8]; Wei et al.'s magnetically adjustable "ON–OFF" Fe_3O_4@PDA hydrogel for traumatic brain injury (TBI) exhibits a remote stiffening response under a magnetic field to stimulate TRPV4-mediated Ca^{2+} signaling, thereby enhancing BMSC neuronal differentiation, axonal regeneration, synapse formation, and spatial learning capabilities [9]; Delavar et al.'s self-sustaining bilayer piezoelectric conduit for sciatic nerve (PNS) repair employs $BaTiO_3$-doped aligned PCL fibers to elicit endogenous electrical signals, incorporates an outer PAG nanocomposite for structural and conductive reinforcement, and utilizes curcumin-infused

alginate within the lumen for prolonged anti-inflammatory effects, collectively facilitating axonal regrowth and functional recovery [10]; and Zhang et al.'s $Ti_3C_2T_x$ MXene–Matrigel composite for cochlear/hearing interventions establishes a conductive organoid microenvironment that activates mTOR–HIF1α signaling pathways to induce $Atoh1^+$ progenitor cell maturation into electrophysiologically proficient $Myo7a^+$ hair cells and functional reinnervation with spiral ganglion neurons. [11]

Conclusions: Conductive nanocomposite hydrogels combine electrical conductivity with antioxidant, immunomodulatory, and controlled-release functions to counter oxidative stress, suppress inflammation, and restore bioelectrical signaling. They use aligned, magnetically responsive and self-powered systems to guide axons and deliver on-demand stimulation. By integrating electrical, topographical, and biochemical cues, stimuli-responsive CNHs enhance stem-cell differentiation and functional neural recovery.

References:

[1] Moskow J, Ferrigno B, Mistry N, Jaiswal D, Bulsara K, Rudraiah S, Kumbar SG. Review: Bioengineering approach for the repair and regeneration of peripheral nerve. Bioact Mater 2019;4:107–13. https://doi.org/10.1016/j.bioactmat.2018.09.001.

[2] Zhou C, Wu T, Xie X, Song G, Ma X, Mu Q, Huang Z, Liu X, Sun C, Xu W. Advances and challenges in conductive hydrogels: From properties to applications. Eur Polym J 2022;177:111454. https://doi.org/10.1016/j.eurpolymj.2022.111454.

[3] Zhu R, Sun Z, Li C, Ramakrishna S, Chiu K, He L. Electrical stimulation affects neural stem cell fate and function in vitro. Exp Neurol 2019;319:112963. https://doi.org/10.1016/j.expneurol.2019.112963.

[4] Heng BC, Bai Y, Li X, Meng Y, Zhang X, Deng X. Signaling pathways implicated in enhanced stem/progenitor cell differentiation on electroactive scaffolds. Smart Mater Med 2022;3:4–11. https://doi.org/10.1016/j.smaim.2021.11.003.

[5] Zhang W, Yang Y, Cui B. New perspectives on the roles of nanoscale surface topography in modulating intracellular signaling. Curr Opin Solid State Mater Sci 2021;25:100873. https://doi.org/10.1016/j.cossms.2020.100873.

[6] Tricco AC, Lillie E, Zarin W, O'Brien KK, Colquhoun H, Levac D, Moher D, Peters MDJ, Horsley T, Weeks L, Hempel S, Akl EA, Chang C, McGowan J, Stewart L, Hartling L, Aldcroft A, Wilson MG, Garritty C, Lewin S, Godfrey CM, Macdonald MT, Langlois EV, Soares-Weiser K, Moriarty J, Clifford T, Tunçalp Ö, Straus SE. PRISMA Extension for Scoping Reviews (PRISMA-ScR): Checklist and Explanation. Ann Intern Med 2018;169:467–73. https://doi.org/10.7326/M18-0850.

[7] Ouzzani M, Hammady H, Fedorowicz Z, Elmagarmid A. Rayyan—a web and mobile app for systematic reviews. Syst Rev 2016;5:210. https://doi.org/10.1186/s13643-016-0384-4.

[8] Li Z, Wang X, Zhao Z, Liu Y. A conductive piezoelectric hydrogel combined with perampanel and wireless electrical stimulation for spinal cord injury repair. Chem Eng J 2024;493:152238. https://doi.org/10.1016/j.cej.2024.152238.

[9] Wei D, Zeng M, Su B, Zhang Y, Ding J, Wu C, Sun J, Zhou L, Yin H, Fan H. Magnetic on–off manipulated matrix mechanic vibration to enhance cell clutches-reinforcement and Ca2+ influx facilitating BMSCs neural differentiation and TBI repair. Chem Eng J 2024;484:149521. https://doi.org/10.1016/j.cej.2024.149521.

[10] Delavar F, Mohseni M, Jahandideh A, Khajehmohammadi M, Najmoddin N. Piezoelectric bilayer fibrous conduit with gellan/curcumin encapsulated alginate infilling for promotion of sciatic nerve regeneration in the rat models. Int J Biol Macromol 2025;286:137833. https://doi.org/10.1016/j.ijbiomac.2024.137833.

[11] Zhang Z, Gao S, Hu Y-N, Chen X, Cheng C, Fu X-L, Zhang S-S, Wang X-L, Che Y-W, Zhang C, Chai R-J. Ti3C2TxMXene Composite 3D Hydrogel Potentiates mTOR Signaling to Promote the Generation of Functional Hair Cells in Cochlea Organoids. Adv Sci 2022;9:2203557. https://doi.org/10.1002/advs.202203557.

SC-OP11 DEVELOPMENT AND CHARACTERIZATION OF ELECTROSPUN PLA/PCL SCAFFOLDS CO-LOADED WITH SILVER SULFADIAZINE AND SUPERCRITICAL-EXTRACTED CLOVE OIL FOR WOUND HEALING APPLICATIONS

Tubanur Avcı[1], Rabia Sulutaş[1], Fatih Mehmet Yıldız[1], Melek Beyza Reyhanoğlu[1], Şevval Güneş[1], Yusuf Ülker[1], Sümeyye Cesur Satıç[1], Canan Doğan[1], Oğuzhan Gündüz[1]

[1] Marmara University, Nanotechnology and Biomaterials Application and Research Center (NBUAM), Istanbul, Türkiye

Abstract: *Chronic wounds, particularly infected burn wounds, pose significant healthcare challenges due to complications like biofilm formation and antibiotic resistance. This study aimed to develop and comprehensively characterize a multifunctional nanofibrous wound dressing by combining the biocompatible polymers Polylactic Acid (PLA) and Poly(ε-caprolactone) (PCL) with the natural antimicrobial agent clove oil (CLV) and the antibacterial drug silver sulfadiazine (AgSD). Four groups of nanofibrous mats were fabricated via electrospinning: PLA/PCL (75:25 ratio), PLA/PCL/CLV (15% v/v), PLA/PCL/AgSD (0.2% w/v), and a co-loaded PLA/PCL/CLV/AgSD. The clove oil, extracted using supercritical fluid extraction (SFE-CO_2), was confirmed by GC-MS to be predominantly composed of eugenol (67.96%). The scaffolds were characterized for their morphology (SEM), chemical structure (FTIR), thermal properties (DSC, TGA), crystallinity (XRD), mechanical strength, swelling/degradation behavior, in vitro drug release, antimicrobial efficacy, and biocompatibility.*

SEM analysis revealed uniform, bead-free nanofibers with average diameters ranging from approximately 617 nm to 781 nm. FTIR confirmed the successful incorporation of both CLV and AgSD within the PLA/PCL polymer blend. Mechanical testing demonstrated that AgSD increased tensile strength (2.25 MPa) but reduced elongation (59.64%), whereas CLV acted as a plasticizer, enhancing flexibility (92.60% strain at break). The co-loaded (CLV/AgSD) fibers exhibited a balanced mechanical profile suitable for wound dressing applications. Antimicrobial assays showed that the clove extract possessed a Minimum Inhibitory Concentration (MIC) of 11 mg/ml against S. aureus, E. coli, and P. aeruginosa. The AgSD-loaded and co-loaded CLV-AgSD fibers both achieved approximately 96% bacterial growth inhibition. Notably, the combined CLV-AgSD scaffold demonstrated the highest synergistic biofilm inhibition (95%) against P. aeruginosa PA01. Biocompatibility studies using Human Dermal Fibroblasts (HDF) showed that CLV-containing groups significantly promoted cell proliferation, with the PLA/PCL/CLV group reaching 292.64% viability on day 1. While AgSD alone initially reduced viability, all formulations, including the co-loaded group (239.80% on day 1), demonstrated excellent cell compatibility and proliferation by day 3.

In conclusion, the electrospun PLA/PCL/CLV/AgSD nanofibrous scaffold integrates the structural and mechanical benefits of the polymer blend with the potent, synergistic antimicrobial and antibiofilm activities of clove oil and silver sulfadiazine. This combination, along with its high biocompatibility, presents a promising advanced biomaterial for effective burn wound healing and chronic wound management.

SC-OP12 A HYBRID APPROACH TO PROMOTE NEURAL REGENERATION THROUGH LAYERED BIOMATERIAL DESIGN

Esin Şahsenem Karakurt[1], Tuğba Kirim[1], Dilara Odabaşi[1], Ayşe Betül Bingöl[*], Büşra Oktay[1], Fatih Çiftçi[2], Cem Bulent Üstündağ[1]

[1]Yıldız Technical University, Faculty of Chemistry and Metallurgy, Department of Bioengineering, Istanbul 34220, Turkıye

[2]Faculty of Engineering, Department of Biomedical Engineering, Fatih Sultan Mehmet Vakıf University, Istanbul 34015, Turkıye

Abstract: *Spinal cord injury leads to severe neurological impairment because of the limited regenerative capacity of neural tissue. In this study, a dual-layer wound dressing was developed to integrate mechanical reinforcement with bioactive stimulation for potential neural tissue regeneration. The bottom layer, composed of PLA/HA (polylactic acid/hydroxyapatite), was produced via a modified melt extrusion method, while the upper layer of PCL/GO/SV (polycaprolactone/graphene oxide/sodium valproate) was fabricated through electrospinning to create a nanofibrous architecture supporting cell adhesion and controlled drug release. The scaffold was characterized using FTIR, SEM, and DSC analyses to determine its structural and thermal properties, and cytocompatibility was assessed through MTT assays. The results confirmed the successful fabrication of the bilayer scaffold with appropriate chemical composition, thermal stability, and high cell viability. Further studies, including tensile, drug release, and swelling–degradation analyses, will be performed to evaluate the scaffold's mechanical behavior and long-term performance. These findings highlight the potential of this bilayer construct as a multifunctional biomaterial platform for spinal cord repair and neural regeneration.*

Keywords: Controlled drug release, Biocompatibility, Morphological characterization, Thermomechanical behavior, Spinal cord injury

Introduction: Spinal cord injuries (SCIs) remain one of the most challenging conditions in regenerative medicine, often leading to irreversible functional loss [1, 2]. The development of multifunctional scaffolds that combine structural stability and biological activity is critical for promoting neuronal healing [3]. Biodegradable polymers such as PLA and PCL, enhanced with inorganic and conductive additives like HA and GO, have attracted significant attention for their ability to mimic the extracellular matrix and stimulate regeneration [4, 5]**.**

Experimental and/or Modelling: A bilayer scaffold was fabricated by integrating two complementary fabrication methods. The PLA/HA [6] layer was produced by a modified melt extrusion technique ensuring structural strength and bioactivity. The PCL/GO/SV layer was fabricated via electrospinning to provide a nanofibrous surface favorable for neural attachment and drug release. The structure was characterized using FTIR, SEM, and DSC testing, while MTT assays were performed to assess cytocompatibility.

[*] Corresponding author: betulbngla@gmail.com

Results and discussions : FTIR analysis verified the presence of characteristic functional groups of PLA, PCL, HA, and GO, confirming the successful incorporation of the additives without the formation of new chemical bonds and indicating structural stability of the composite layers. SEM imaging was performed to examine the surface morphology and layer interface of the scaffold. DSC results showed that the thermal transitions of the polymers were preserved, demonstrating the thermal stability of the material. MTT assays confirmed high fibroblast viability, indicating that the fabricated scaffold is cytocompatible and suitable for further biological evaluation. Overall, the obtained data validate the successful fabrication of the bilayer structure and its potential use in neural tissue engineering applications.

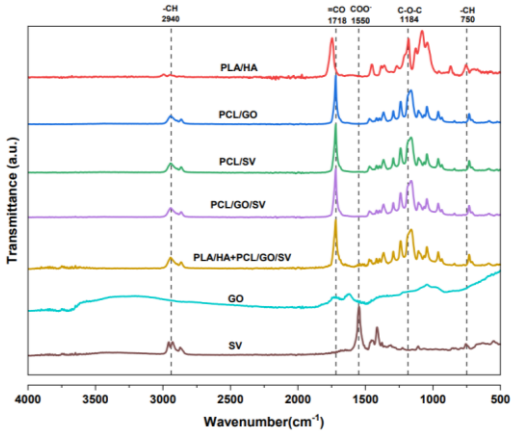


Fig. 1. FTIR spectra of layered biomaterial structures.

Conclusions: A bilayer PLA/HA–PCL/GO/SV scaffold was successfully fabricated and characterized using FTIR, DSC, SEM, and MTT analyses. Further studies including tensile, drug release, and swelling–degradation tests will be conducted to evaluate its mechanical and biofunctional performance.

References:

[1] Gao, Y., Li, X., & Wang, J. (2024). Biomaterials targeting the microenvironment for spinal cord repair. *Frontiers in Cellular Neuroscience*.

[2] Zhu, S., et al. (2025). Biomaterial-based strategies: a new era in spinal cord tissue engineering. *Journal of Tissue Engineering*, 16, 118–132.

[3] Liao, Z. (2025). Research progress on biomaterials for spinal cord repair. *International Journal of Nanomedicine*.

[4] Yang, Z., et al. (2024). Medical applications and prospects of polylactic acid-based materials. *Acta Biomaterialia*, 165, 300–314.

[5] Altunordu Kalaycı, Ö., & Arslan, H. (2023). Synthesis of polymer hybrid nanomaterials containing silver nanoparticles and the effect of nanoparticles on methylene blue reduction. *Düzce University Journal of Science and Technology*, 11(3), 1349-1364.

[6] Ustundag, C. B. (2016). Fabrication of porous hydroxyapatite–carbon nanotubes composite. Materials Letters, 167, 89–92.

SC-OP13 GRAPHENE OXIDE REDUCTION METHODS: PROPERTIES, APPLICATIONS, AND BIOMEDICAL RELEVANCE

Ayse Betul Bingol[1*], Busra Oktay[1], Alpay Kose[1], Israa F Abdulazez[1,2], Cem Bulent Ustundag[1,3]

[1]Yildiz Technical University, Faculty of Chemistry and Metallurgy, Department of Bioengineering, Istanbul, Turkey

[2]University of Baghdad Al-Khwarizmi College of Engineering Biomedical Engineering Departments, Baghdad, Iraq

[3] Health Biotechnology Joint Research and Application Center of Excellence, Istanbul 34220, Turkey

Abstract: *Back in the early 2010s, reduced graphene oxide (rGO) began to draw attention as an oddly balanced material, part conductor, part bio-friendly platform. Reduced graphene oxide (rGO) has emerged as a key nanomaterial bridging the gap between conductive carbon frameworks and biologically compatible systems. Over time, it gradually became clear that this mix of high conductivity, surface activity, and compatibility with cells wasn't a coincidence but a controllable outcome of its reduction pathway. This review summarizes the most relevant advances in the synthesis and reduction of graphene oxide (GO) using chemical, thermal, electrochemical, hydrothermal, microwave-assisted, and environmentally friendly "green" approaches. Each method offers distinct advantages in controlling the oxygen content, crystallinity, and electrical conductivity of rGO. Special attention is given to how reduction pathways influence biocompatibility and surface chemistry, which are essential for biomedical applications. The review also discusses the structure–property–function relationship of rGO and its growing role in tissue engineering, drug delivery, biosensing, and photothermal therapy. Although significant progress has been made in understanding reduction mechanisms and material optimization, there is still no universal consensus on the ideal synthesis route. The future of rGO research lies in integrating green chemistry principles with scalable production strategies, ultimately enabling its safe and sustainable use in advanced biomedical and electronic systems.*

Keywords: Reduced graphene oxide, green synthesis, electrical conductivity, biocompatibility, biomedical applications

Introduction: Graphene oxide (GO) sits at an interesting intersection of chemistry and engineering. It carries oxygen-rich groups that make it dispersible and reactive, yet those same groups strip away its natural conductivity (Candotto Carniel et al., 2021). Reducing GO back toward graphene, but not all the way, gives rise to reduced graphene oxide, rGO-a halfway house that preserves just enough oxygen to interact with biological molecules. Over the past decade, researchers have learned that this "partial reduction" is where most of the magic happens (Syama & Mohanan, 2019). Conductivity returns, mechanical strength improves, and the surface becomes just polar enough to host proteins, drugs, and even living cells. The motivation behind this study was simple: to unpack how different reduction methods change the internal structure of rGO, and how these subtle changes ripple outward into biomedical performance (Bellier et al., 2022; Reina et al., 2017).

Experimental and/or Modelling: There's no single formula for making rGO; every method carries its own rhythm. Chemical routes rely on reducers such as hydrazine, sodium

* Corresponding author:

borohydride, or the gentler ascorbic acid. They're efficient, sometimes too much so, stripping oxygen groups so aggressively that little room remains for later functionalization. Thermal reduction, on the other hand, is all about heat-temperatures soaring past 800 °C under inert gas. It works, but at a cost: high energy consumption and lost surface chemistry. Green synthesis entered the scene as a response to this problem, using plant extracts, vitamins, and amino acids to create mild, eco-friendly pathways. Electrochemical and microwave-assisted reductions added their own twists, each giving precise control or rapid heating. In this comparison, emphasis was placed not just on conductivity but also on reproducibility, environmental footprint, and the biocompatibility of the final product.

Results and discussions: As expected, no single reduction path dominates. Thermally reduced rGO displayed the highest conductivity, sometimes approaching that of pristine graphene, but it also showed the least functional groups, which are vital for biomedical binding (Farah et al., 2020). Green and electrochemical methods produced materials that were somewhat less conductive yet far more compatible with living systems (Cherian et al., 2019; Vijayaram et al., 2024). In XRD data, the GO peak near 11° shifted toward 25°, signaling restoration of the graphitic lattice, while FTIR spectra confirmed the fading of C-O-C and OH bands (Das et al., 2024). Biocompatibility tests show that mild reduction enhances cellular attachment and viability, confirming its promise for regenerative medicine (Bellier et al., 2022; Reina et al., 2017).

Conclusions: Among available reduction strategies, green and electrochemical pathways appear most balanced in terms of efficiency, safety, and biomedical potential (Rehman et al., 2025; Vijayaram et al., 2024). Their ability to yield conductive yet biocompatible rGO ensures continuing relevance in future bio-nanomaterial design.

References:

[1] Candotto Carniel, F., Fortuna, L., Zanelli, D., Garrido, M., Vázquez, E., González, V. J., Prato, M., & Tretiach, M. (2021). *Graphene environmental biodegradation: Wood-degrading and saprotrophic fungi oxidize few-layer graphene.* **Journal of Hazardous Materials, 414**, 125553. https://doi.org/10.1016/j.jhazmat.2021.125553

[2] Syama, S., & Mohanan, P. V. (2019). *Comprehensive application of graphene: Emphasis on biomedical concerns.* **Nano-Micro Letters, 11**(1), 23. https://doi.org/10.1007/s40820-019-0237-5

[3] Bellier, N., Baipaywad, P., Ryu, N., Lee, J. Y., & Park, H. (2022). *Recent biomedical advancements in graphene oxide- and reduced graphene oxide-based nanocomposite nanocarriers.* **Biomaterials Research, 26**(1), 1–23. https://doi.org/10.1186/s40824-022-00313-2

[4] Farah, S., Farkas, A., Madarász, J., & László, K. (2020). *Comparison of thermally and chemically reduced graphene oxides by thermal analysis and Raman spectroscopy.* **Journal of Thermal Analysis and Calorimetry, 142**(1), 331–337. https://doi.org/10.1007/s10973-020-09719-3

[5] Cherian, R. S., Sandeman, S., Ray, S., Savina, I. N., Ashtami, J., & Mohanan, P. V. (2019). *Green synthesis of Pluronic stabilized reduced graphene oxide: Chemical and biological characterization.* **Colloids and Surfaces B: Biointerfaces, 179**, 94–106. https://doi.org/10.1016/j.colsurfb.2019.03.043

[6] Das, P., Ibrahim, S., Chakraborty, K., Ghosh, S., & Pal, T. (2024). *Stepwise reduction of graphene oxide and studies on defect-controlled physical properties.* **Scientific Reports, 14**(1), 1–10. https://doi.org/10.1038/s41598-023-51040-0

[7] Bellier, N., Baipaywad, P., Ryu, N., Lee, J. Y., & Park, H. (2022). *Recent biomedical advancements in graphene oxide- and reduced graphene oxide-based nanocomposite nanocarriers.* **Biomaterials Research, 26**(1), 1–23. https://doi.org/10.1186/s40824-022-00313-2

[8] Reina, G., González-Domínguez, J. M., Criado, A., Vázquez, E., Bianco, A., & Prato, M. (2017). *Promises, facts, and challenges for graphene in biomedical applications.* **Chemical Society Reviews, 46**(15), 4400–4416. https://doi.org/10.1039/c7cs00363c

[9] Rehman, N., Pandey, A., & Pandey, A. (2025). *Thermal reduction synthesis approach of reduced graphene oxide for label-free and prompt immunosensing of Salmonella enterica via electrochemical techniques.* **Sensing and Bio-Sensing Research, 48**, 100789. https://doi.org/10.1016/j.sbsr.2025.100789

[10] Vijayaram, S., Razafindralambo, H., Sun, Y. Z., Vasantharaj, S., Ghafarifarsani, H., Hoseinifar, S. H., & Raeeszadeh, M. (2024). *Applications of green synthesized metal nanoparticles — A review.* **Biological Trace Element Research, 202**(1), 360–386. https://doi.org/10.1007/s12011-023-03645-9

BOOK OF ABSTRACTS

SICHEM – 2025

C – Biomaterials and composites in chemical and biochemical applications (BCCBA)

3. Poster presentations

SC-P01 BRUSHITE VS. MONETITE: OPTIMIZING CALCIUM PHOSPHATE SELECTION FOR 3D-PRINTED BONE SCAFFOLDS

Andreea Trifan[1,2*], Cristina Busuioc[1], Eduard Liciu[2], Andrei-Silviu Nedelcu[3], Mihai Dragomir[2], Doru-Daniel Cristea[2,4], Ciprian-Ștefan Mateescu[2,4], Adela Banciu[3], Gabriela Toader[5], Aurel Diacon[5]

[1] Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology Politehnica Bucharest, RO-011061 Bucharest, Romania

[2] 3D Printing Laboratory, Center of Innovation and e-Health, Carol Davila University of Medicine and Pharmacy, RO-020021 Bucharest, Romania

[3] Faculty of Medical Engineering, National University of Science and Technology Politehnica Bucharest, RO-011061 Bucharest, Romania

[4] Reorom Laboratory, Hydraulics Department, Power Engineering Faculty, National University of Science and Technology Politehnica Bucharest, RO-060042 Bucharest, Romania

[5] Military Technical Academy "Ferdinand I", RO-050141 Bucharest, Romania

Abstract: *This study presents a comprehensive comparison between brushite (dicalcium phosphate dihydrate) and monetite (dicalcium phosphate anhydrous) powders incorporated into 3D-printed composite hydrogels for bone tissue engineering applications. Both calcium phosphate (CaP) phases were integrated into alginate-gelatin bioinks to develop bioactive scaffolds with enhanced mechanical and biological properties. The comparative analysis revealed distinct performance characteristics between the two CaP phases, with brushite-containing scaffolds demonstrating superior initial bioactivity and 15-25% increased mechanical stability, while monetite-incorporated scaffolds exhibited more sustained degradation profiles and longer-term structural support.*
Key words: brushite, monetite, calcium phosphates, bone tissue engineering, composite hydrogels.

Introduction: The development of bioactive hydrogel scaffolds that can promote osteogenesis while providing mechanical support remains a significant challenge in regenerative medicine [1]. Among CaP phases, brushite and monetite offer distinct advantages due to their different solubility profiles and bioactivity characteristics [2]. This research focuses on the synthesis and characterization of composite scaffolds incorporating CaP for bone tissue engineering applications.

Experimental: *Reagents*: Sodium alginate, gelatin, calcium chloride, CaP powder precursors were obtained from commercial sources.

Scaffold fabrication: Composite hydrogels were prepared by incorporating synthesized 1-5% w/v CaP [3] into alginate-gelatin matrices. 3D printing was performed using extrusion-based bioprinting with optimized printing parameters.

Characterization methods: Scaffolds were evaluated through morphological analysis, mechanical testing, *in vitro* mineralization study, while cell viability was assessed using LIVE/DEAD assay with preosteoblast cell lines.

* Corresponding author: andreea.trifan@stud.fim.upb.ro.

Results and discussions: The incorporation of both CaP phases significantly enhanced scaffold properties compared to pure hydrogel controls, regarding print fidelity, scaffold stability and swelling behaviour. Mechanical testing revealed 15-25% improvement in compressive strength for CaP scaffolds. Monetite scaffolds exhibited more sustained degradation profiles, maintaining structural integrity over extended periods due to its stability at physiological pH, as shown in Fig. 1. LIVE/DEAD assay confirmed biocompatibility of both formulations, while mineralization studies revealed distinct kinetics, with brushite promoting faster initial mineral deposition.

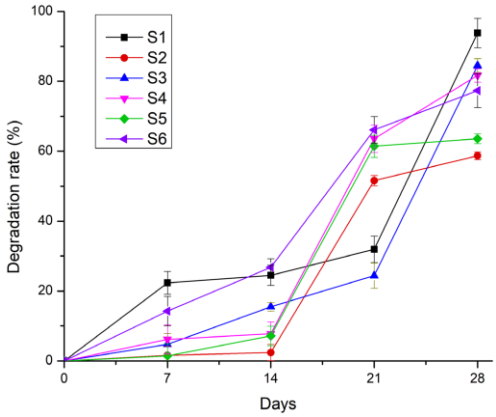


Fig. 1. Degradation rate of the 3D-printed scaffolds S1–S6 after 7, 14, 21, and 28 days.

Conclusions: This work studied 3D printed composite scaffolds based on polymers and CaP, with both inorganic phases enhancing the construct properties.

References:

[1] Trifan, A.; Liciu, E.; Nedelcu, A.S.; Dragomir, M.; Cristea, D.D.; Mateescu, C.Ș.; Nițulescu, D.A.; Cîrstea, C.A.M.; Banciu, A.; Toader, G.; Diacon, A., Busuioc, C. Effect of Phosphate Phase Incorporation on 3D-Printed Hydrogel Scaffolds: Towards Customizable Bone Graft Materials. *Gels* **2025**, *11*, 665. https://doi.org/10.3390/gels11080665.

[2] Boanini, E.; Pagani, S.; Tschon, M.; Rubini, K.; Fini, M.; Bigi, A. Monetite vs. Brushite: Different Influences on Bone Cell Response Modulated by Strontium Functionalization. *J. Funct. Biomater.* **2022**, *13*, 65. https://doi.org/10.3390/jfb13020065.

[3] Teterina, A.Y.; Smirnov, I.V.; Fadeeva, I.S.; Fadeev, R.S.; Smirnova, P.V.; Minaychev, V.V.; Kobyakova, M.I.; Fedotov, A.Y.; Barinov, S.M.; Komlev, V.S. Octacalcium Phosphate for Bone Tissue Engineering: Synthesis, Modification, and In Vitro Biocompatibility Assessment. *Int. J. Mol. Sci.* **2021**, *22*, 12747. https://doi.org/10.3390/ijms222312747.

SC-P02 MICROSTRUCTURED MATERIALS WITH APPLICATIONS IN THE DEVELOPMENT OF PORTABLE BIOSENSORS

Gabriela-Alexandra Rotaru [1*], Oana-Daciana Botta[2],
Victor-Constantin Diculescu[2], Cristina Busuioc [1]

[1] National University of Science and Technology Politehnica Bucharest, 1-7 Polizu Street, Bucharest, Romania, RO-011061

[2] National Institute of Materials Physics, 405A Atomistilor Street, Bucharest-Magurele, Ilfov, Romania, RO-077125

Abstract: The biosensor architecture combines electrospun polymethyl methacrylate (PMMA) nanofibres with a thin layer of gold deposited by magnetron sputtering, resulting in a conductive and mechanically stable electrode network. The porous PMMA nanofibre web serve as a high-surface-area scaffold that enhances enzyme immobilization and electron transfer, while the gold coating provides electrical conductivity and biocompatibility. The metalized nanofibres were thermally transferred onto chromatographic paper, forming a lightweight and flexible electrochemical cell. Additionally, microfluidic channels were patterned through 3D printing and thermal treatment to ensure precise control of fluid transport and sample distribution.

Material characterization using scanning electron microscopy (SEM) and UV-Vis spectroscopy confirmed the uniformity of the electrospun structures and controlled metallic layer deposition. SEM images showed continuous, interconnected fibres with uniform gold coverage, while UV-Vis analysis indicated suitable transparency matching the desired film thickness. Electrochemical studies (cyclic voltammetry and amperometry) revealed stable redox behaviour and strong electrocatalytic activity towards hydrogen peroxide (H_2O_2), the by-product of glucose oxidation by glucose oxidase (GOx). The biosensor achieved a detection limit of ~13 μM, suitable for glucose monitoring in non-invasive fluids such as sweat or saliva.

The developed system is reproducible, easy to fabricate, and compatible with miniaturized and disposable designs, meeting the functional requirements for future wearable glucose monitoring technologies.

Keywords: Microstructured materials, Electrospinning, Gold sputtering, Glucose detection, Electrochemical sensing, Portable biosensor.

References:

[1] C. Busuioc, A. Evanghelidis, A. Galatanu, I. Enculescu, Sci. Rep. **2016**, *6*, 34584.
[2] D. Botta, I. Enculescu, C. Balan, V.C. Diculescu, *Curr. Opin. Electrochem.* **2023**, *42*, 101418.
[3] D. Botta, M. Beregoi, I.A. Cepleanu-Pascu, D.N. Crisan, A.M. Ignat, E. Matei, I. Enculescu, V.C. Diculescu, *Cell Reports Phys. Sci.* **2025**, *6*, 102781

* Corresponding author:

SC-P03 LASER SURFACE MODIFICATION OF TITANIUM - A WAY TO IMPROVE ITS BIOLOGICAL PROPERTIES

J. Kisała[1*], A. Barylyak[2], P. Krzemiński[1], R. Wojnarowska-Nowak[1], B. Cieniek[1], M. Kus-Liśkiewicz[3], Y. Bobitski[1]

[1]Faculty of Exact and Technical Sciences, University of Rzeszow, Pigonia 1str., 35-310 Rzeszow, Poland

[2]Danylo Halytsky Lviv National Medical University, Pekarska str. 69, Lviv, 79010, Ukraine

[3]Faculty of Biotechnology, University of Rzeszow, Rejtana 16 c, 35-959 Rzeszow, Poland

Abstract: *This work aims to demonstrate the possibility of obtaining a functionally orientated surface of titanium implant elements with a specific architecture with specific bacteriological and photocatalytic properties. Femtosecond laser-generated surface structures, such as laser-induced periodic surface structures (LIPSS, wrinkles), grooves, and spikes on titanium, have been physico-chemically characterized. The photocatalytic activity of the laser produced surfaces produced was tested in the degradation of methylene blue (MB). Features related to the size, shape, and distribution of the roughness patterns were found to influence the adhesion of the bacterial strain on different surfaces. On the laser-structurised surface, the adhesion of Escherichia coli bacteria were reduced by 80% compared to an untreated reference surface.*

Key words: Ultra-short pulsed laser treatment, Reduced bacterial adhesion, Photocatalytic activity

Introduction: Titanium and its alloys are most widely used for load-bearing metal implants due to their good tolerance by living tissues as well as their capability of osseointegration promotion [1]. Key challenges are sub-optimal bone integration in compromised bone conditions and in the presence of a persistent oral microbial biofilm [2]. The laser's ability to precisely change the surface features of a material and hence its interactions with the surroundings allows for improving the material's behaviour with biological systems.

Experimental and/or Modelling: *Surface preparation*: The structure generation was carried out using a Pharos P-20 femtosecond laser system that provides femtosecond pulses (τ = 213 fs) at a central wavelength of 1030 nm with a spectral width of 15 nm, M2 ≃ 1.1. The laser beam was focused on the titanium surface at a spot diameter of 10.4 μm (at level $1/e^2$). A scanning mode with various overlaps was used for irradiation. *Antibacterial tests: E. coli* cells were seeded on the titanium disc and were incubated for 4 h. Next, the disc was carefully rinsed to remove the unattached cells and the adherent cells were fixed in 2.5% glutaraldehyde for 60 min. After this, the discs were dehydrated in 30%, 50%, 70%, 85% and 95% ethanol for 5 min, respectively, and 100% ethanol for 20 min.

Results and discussions: Depending on the laser parameters, the obtained structures differ in roughness, wettability, chemical composition, photocatalytic activity, biocompatibility, and antibacterial properties [3]. Surface modification using laser pulses

* Corresponding author: jkisala@ur.edu.pl

of varying energies promotes the formation of diverse patterns on the surface and alters its chemical composition. The samples were analysed by Raman spectroscopy to determine the composition of the surface layer, especially the presence of the titanium oxides or other oxides. The results showed the presence of titanium oxides on the surface of samples A_1 and A_2. It was not observed in samples A_3 (LIPSS) and A_4 (control). The photocatalytic activity was observed only for A_1 and A_2. It is involved with the presence of oxide layer on these surfaces. A decrease in the number of bacteria cells was observed for the A_1, A_2, and A_3 discs, compared to the unstructured Ti disc, A_4 (Fig. 1A). For each of the modified Ti discs, a reduction in cell population (range between 79 and 87%) was observed.

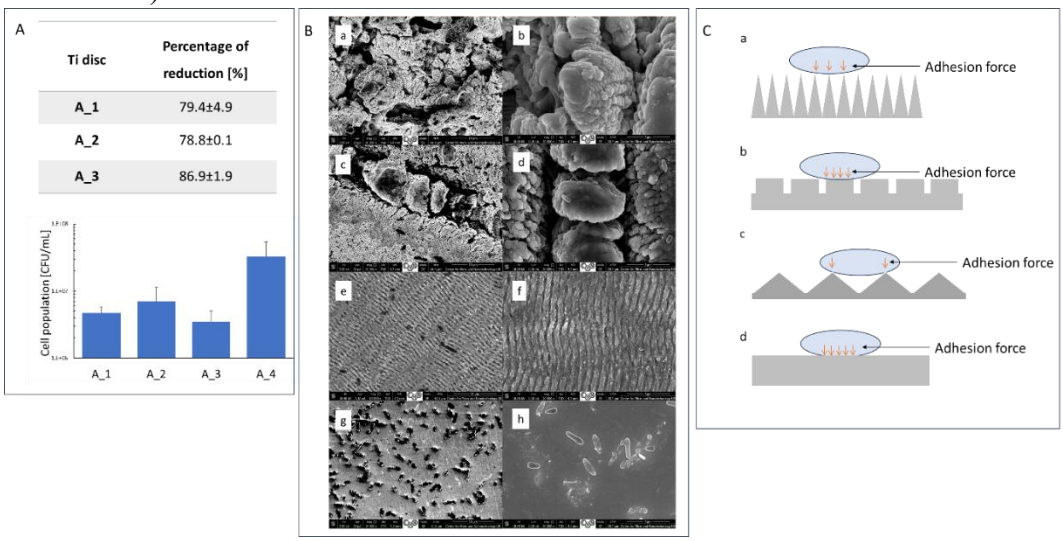


Fig. 1 (**A**) The antibacterial activity of various titanium discs is shown as the number of CFU and percentage reduction in the cell population. The error bars indicated the standard deviation of two independent experiments, the statistical analysis was performed with Dunett´s multiple comparison test with GraphPad Prism. (**B**) SEM images of *E. coli* bacteria cells on surfaces A_1 (a), A_2 (c), A_3 (e), A_4 (g) (before Au spraying), A_1 (b), A_2 (d), A_3 (f), A_4 (h) (after Au spraying). (**C**) Schematic diagram of the bacteria-Surface interaction—A_1 (a), A_2 (b), A_3 (c), A_4 (d)

Conclusions: Femtosecond-laser processing of Ti surfaces is a convenient single-step process of surface texturing that enables the generation of various patterns depending on laser parameters. The LIPSS structures showed excellent properties in inhibiting *E. coli* adhesion. However, the remaining structures also have very good antimicrobial properties and additionally demonstrate photocatalytic activity. The results indicated that laser texturing can be an effective method for enhancing implant surfaces and reducing the risks of implant-associated infections.

References:

[1] Jemat A, Ghazali MJ, Razali M, Otsuka Y., *Biomed Res Int*. **2015**, 2015, 791725.
[2] Diz P, Scully C, Sanz M. J Dent. 2013 Mar;41(3):195-206.
[3] Barylyak A, Wojnarowska-Nowak R, Kus-Liśkiewicz M, Krzemiński P, Płoch D, Cieniek B, Bobitski Y, Kisała J. Sci Rep. 2024 Sep 9;14(1):20926.

SC-P04 SYNTHESIS AND CHARACTERIZATION OF Ni NANOSTRUCTURES

R. Lavric[1,2*], R. Grigore[2,3], E. Matei[2], L. Nedelcu[2], C. Busuioc[1], I. Enculescu[2]

[1] Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology Politehnica Bucharest, RO-060042 Bucharest, Romania

[2] National Institute of Materials Physics, Atomistilor 405A, 077125 Magurele, Ilfov, Romania

[3]Faculty Of Physics, University of Bucharest, 077125 Magurele, Ilfov, Romania

Abstract: *Nickel (Ni) nanostructures exhibit unique physico-chemical properties, making them attractive for applications in catalysis, magnetic storage, and sensing. This study reports the fabrication of Ni nanopillars and nanowires by electrochemical deposition within anodic aluminum oxide (AAO) membranes produced via hard anodization, allowing precise morphological control. The nanostructures were characterized by using SEM for morphology, EDX for elemental composition, and XRD for crystallographic analysis. The results confirm that deposition within AAO templates yields well-defined Ni nanostructures with tunable properties, establishing clear correlations between synthesis parameters, and highlighting their potential for use in magnetic sensing, nanoelectronics, and data storage applications.*

Key words: Ni nanowires, nanopillars, AAO membranes, electrochemical deposition

Introduction: Nickel (Ni) nanowires with longitudinal magnetization exhibit stable magnetic behavior, tunable anisotropy, and good conductivity, making them ideal for miniaturized magnetic sensors [1]. Their elongated structure enhances magnetic field detection, useful in biomedical, industrial, and navigation applications [2]. Owing to recent fabrication advances, Ni nanowires are also promising for spintronics, magnetic memory, and other emerging technologies.

Experimental: *Reagents:* oxalic acid, nickel (II) sulfate hexahydrate, nickel chloride hexahydrate, boric acid

Synthesis of anodic aluminum oxide membranes: High-purity aluminum discs were ultrasonically cleaned and electropolished, then anodized in oxalic acid solution at 0°C with voltages from 80–120 V. This hard anodization produced alumina membranes with ~120 nm pores diameters and ~60 μm channels lengths.

Electrochemical deposition of Ni nanostructures: Ni nanostructures were electrodeposited using a tree electrodes setup with the AAO membranes covered on one surface with Au as working electrode, and Pt mesh as counter electrode and an Red Rod reference electrode (Radiometer REF201), an aqueous solution of $NiSO_4 \cdot 6H_2O$, H_3BO_3, and $NiCl_2 \cdot 6H_2O$ at room temperature using chronoamperometry at –1 V. Varying the deposition time allowed control of morphology: shorter times (60 s) produced nanopillars, while longer times (600–1500 s) yielded nanowires.

* Corresponding author: roxana.lavric@stud.sim.upb.ro

Results and discussions: The electrochemical deposition of Ni nanostructures was monitored at constant potential to analyze the effects of deposition time and membrane wetting. Figure 1 presents current–time curves for nanowires (a) and nanopillars (b). Each curve shows an initial rapid increase due to polarization, followed by a stable plateau indicating steady growth. For samples without wetting, a sharp current drop suggests irregular and less efficient deposition. In contrast, membranes pre-wetted for 1 h and 2 h show smoother, more stable current profiles. The higher, more electronegative current observed after 2 h of wetting reflects enhanced charge transfer and electrolyte diffusion, leading to more uniform, controlled, and efficient Ni nanostructure growth.

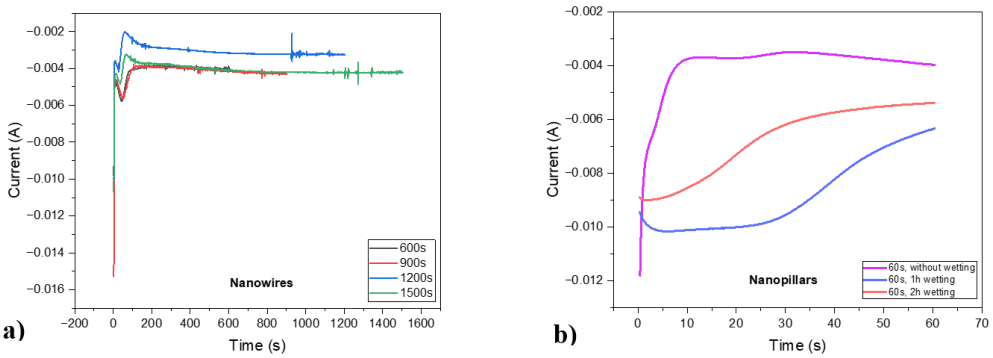


Fig. 1 Deposition curves of Ni nanostructures in the pores of anodic alumina membranes at -1V (I vs. t) to obtain: nanowires (a) and nanopillars (b)

Conclusions: This work examined Ni nanostructures electrodeposited in AAO templates, highlighting the potential for precise nanostructure fabrication.

References:

[1] Tishkevich, D.; Vorobjova, A.; Shimanovich, D.; Kaniukov, E.; Kozlovskiy, A.; Zdorovets, M.; Vinnik, D.; Turutin, A.; Kubasov, I.; Kislyuk, A.; et al. Magnetic Properties of the Densely Packed Ultra-Long Ni Nanowires Encapsulated in Alumina Membrane. *Nanomaterials* **2021**, *11*, 1775. https://doi.org/10.3390/nano11071775

[2] Wang S, Chen K, Wang M, Li H, Chen G, Liu J et al. Controllable synthesis of nickel nanowires and its application in high sensitivity, stretchable strain sensor for body motion sensing. Journal of Materials Chemistry C. **2018**;6(17):4737-4745. https://doi.org/10.1039/c7tc05970a

SC-P05 TiO_2 NANOPARTICLES AS PHOTOCATALYSTS FOR THE DEGRADATION OF THEORGANIC COMPOUNDS

Ana-Maria Fulgheci[1,2], Roxana-Doina Trusca[3], Ludmila Motelica[3,4,5], Cristina Uncu[1,3], Denisa Ficai[1,3,4], Ovidiu-Cristian Oprea[1,3,4], Anton Ficai[1,3,4*]

[1]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7 Polizu St., 011061 Bucharest, Romania

[2]National Research-Development Institute for Industrial Ecology – ECOIND, 57-73 Drumul Podu Dâmboviței, 060652 Bucharest, Romania

[3]National Centre for Micro and Nanomaterials and National Centre for Food Safety, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology POLITEHNICA Bucharest, Spl. Indendentei 313, 060042, Bucharest, Romania

[4]Academy of Romanian Scientists, 3 Ilfov St., 050044, Bucharest, Romania
[5]Research Center for Advanced Materials, Products and Processes, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

Key words: titania, dyes, photocatalysis, wastewater, methylene blue

Introduction: Methylene blue is a cationic synthetic dye that is commonly used as a colorant for paper, cotton, wool, and silk. It is well known that methylene blue is highly persistent in wastewater and challenging to degrade using conventional water treatment [1]. One of the most efficient techniques for breaking down harmful pollutants is photocatalysis, and TiO_2 is the most promising photocatalyst used for their decomposition [2,3]. In this study, we synthesized two different TiO_2 powders using the sol-gel method and evaluated their capacity to photodegrade methylene blue under UV irradiation, considering MB as a model dye being highly persistent and largely used.

Experimental: The two TiO_2 photocatalysts were synthesized using two different titania precursors - titanium isopropoxide (TiO_2 IP) and titanium (triethanolaminato) isopropoxide (TiO_2 NH_2), via the sol-gel method. The samples were calcined at 700°C for 6 hours. The TiO_2 particles were characterized using the following techniques: Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), X-ray diffraction (XRD), Dynamic Light Scattering analysis (DLS) and Zeta potential analysis. The photocatalytic activity was tested under various conditions to determine the optimal operating parameters.

Results and discussions: In the present work, the influence of the following parameters – concentration of the methylene blue solution, amount of catalyst used, pH of the tested solution, irradiation conditions – on the degradation efficiency was tested. For comparison, the tests were also performed on a commercial TiO_2 sample. It was found that the samples synthesized in this work exhibit a photocatalytic activity similar to that of the commercial sample.

Conclusions: The synthesized photocatalysts can be successfully used to degrade emerging pollutants from wastewater, such as dyes, thus avoiding the adverse effects that methylene blue may have on human health and the ecological balance. In our future research we will investigate the effect of incorporating TiO_2 into the pores of mesoporous silica.

Acknowledgements: This work was supported by the Ministry of Education and Research (Ministry of Research, Innovation and Digitization), CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0522, 47PTE/2025.

References:

[1] P.O. Oladoye, T.O. Ajiboye, E.O. Omotola, O.J. Oyewola, Methylene blue dye: Toxicity and potential elimination technology from wastewater, Results in Engineering 16 (2022). https://doi.org/10.1016/j.rineng.2022.100678.

[2] S. Laghrib, C.E. Gherdaoui, O. Belgherbi, N. Benaskeur, M. Boudissa, A. Kanagaraj, N. Aouffa, Photocatalytic degradation of methylene blue using TiO2 nanoparticles synthesized via the sol–gel method in acidic and neutral media, Reaction Kinetics, Mechanisms and Catalysis 138 (2025) 1725–1745. https://doi.org/10.1007/s11144-025-02816-0.

[3] R.S. Dariani, A. Esmaeili, A. Mortezaali, S. Dehghanpour, Photocatalytic reaction and degradation of methylene blue on TiO2 nano-sized particles, Optik (Stuttg) 127 (2016) 7143–7154. https://doi.org/10.1016/j.ijleo.2016.04.026.

SC-P06 DEVELOPMENT OF UV LIGHT SHIELDING MATERIALS BY DEPOSITING IRON-CHELATED NATURAL POLYPHENOLIC COMPOUNDS ON SERICITE

Monica Florentina Raduly*, Valentin Raditoiu, Alina Raditoiu, Adriana Frone, Cristian Nicolae

National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Abstract: *The cosmetics industry requires safe, high-efficacy, and sustainable ingredients for sunscreen and daily UV protection products. This study addresses this need by reporting the development of novel, mineral-based UV light shielding materials achieved by functionalizing sericite with iron-chelated natural polyphenolic compounds. Sericite, a pure, fine-grained mica mineral, was selected as a superior base over common mineral UV filters due to its smooth texture, high lamellar aspect ratio, and excellent compatibility with cosmetic formulations, offering a non-nano, sensory-enhancing alternative[1-3].*

The methodology focused on enhancing both UV protection and cosmetic safety. Natural polyphenols (known for their antioxidant activity and UV absorbance) from Taraxacum officinale were coordinated with iron ions (Fe^{2+}, Fe^{3+}), forming stable, non-toxic metal-phenolic complexes. Polyphenols were extracted in ethanol from fresh flowers through an ultrasonic process. After extraction, the solutions were filtered and concentrated, yielding polyphenol-rich extracts. These extracts were used in complexation reactions by gradually adding metal salt solutions, adjusting the pH from neutral to slightly basic. The resulting metal complexes were deposited on a sericite support (initially activated by an acid treatment) through adsorption processes carried out under controlled temperature and time conditions. Both the metal complexes and the hybrid materials obtained by their deposition on sericite were characterized using specific analytical techniques, including FTIR spectroscopy, UV-Vis spectroscopy, diffuse reflectance spectroscopy, scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). The obtained hybrid materials exhibited enhanced thermal stability, and were tested in dermato-cosmetic formulations by measuring the sun protective factor (SPF).

The analyses showed that the chelation reaction of iron ions took place successfully, the first indication being given by the change in the color of the natural extracts from the initial yellow, to shades of green and black after the addition of metal salts. The hybrid materials obtained by immobilizing the metal complexes onto sericite exhibited high thermal stability and showed lower transmittance values compared to the inorganic support.

The developed sericite/iron-polyphenol composites offer a novel, multifunctional cosmetic ingredient: a highly effective, non-nanoparticle UV filter that simultaneously acts as a natural pigment and provides superior skin-feel. This research establishes an eco-friendly and safe platform for formulating next-generation cosmetic products, advancing the development of highly protective, aesthetically pleasing, and sustainable sun care and daily protective makeup.

Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PED 2024-0838, within PNCDI IV, partial and through INCDCP ICECHIM Bucharest Core Program—ChemNewDeal PN 23.06, within the National Plan for Research, Development and Innovation 2022–2027, project no. PN 23.06.01.01(AQUAMAT).

References:

[1] Pniewska, A.; Kalinowska-Lis, U. A Survey of UV Filters Used in Sunscreen Cosmetics. Appl. Sci. 2024, 14, 3302

[2] Aswini, T.; Dhanusha, K.; Priya, K.; Shalini, R.; Sumithra, S.; Helen W. A short review on natural components in sunscreen. WJBPHS, 2024, 19(01), 218–224

[3] He hailun, Li anqi, Li shiqin, Tang jie, Li li, Xionglidan. Natural components in sunscreens: Topical formulations with sun protection factor (SPF). Biomedicine & Pharmacotherapy 2021, 134, 111161

* Corresponding author: monica.raduly@icechim.ro

SC-P07 NOVEL APPLICATIONS OF COLLAGEN, HYDROXYAPATITE AND POLYPHENOLS – LOADED MCM41 IN BONE TISSUE ENGINEERING

Ovidiu Cristian Oprea [1,2,4,6], Anton Ficai [1,2,4,6], Ludmila Motelica[1,2,6], Denisa Ficai[1,2,4,6], Roxana Trusca[6], Mariana Jian[3], Viorel Nacu[2], Ecaterina Andronescu [2,6]

[1]Research Center for Advanced Materials, Products and Processes, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

[2]Academy of Romanian Scientist, Bucharest, Romania

[3] Laboratory of Tissue Engineering and Cell Cultures, Nicolae Testemițanu State University of Medicine and Pharmacy, Chisinau, Moldova;

[4]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania

[6]National Center for Micro and Nanomaterials, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest, Romania

Abstract: *A versatile nanostructured material used as drug delivery support is represented by the porous materials such as mesoporous silica and due to the good biological and chemical properties represents a good candidate for many applications including bone-related applications [1]. These nanostructures as well as their analogues loaded with the specific biological active agents can be entrapped in the composite materials, including collagen/hydroxyapatite composites (COLL/HA) [2] in order to be used in bone regeneration.*

In this study, Col/HA/MCM-41 were obtained and used in hard or soft tissue engineering, including as drug delivery system. In the first step, mesoporous silica with different characteristics (structure and porosity) loaded with caffeic and gallic acid, were synthesized by the soft-tempting method. In the second steps, Col/HA/MCM-41/BAA were obtained, using the direct mixing of the MCM-41 loaded with biologically active agent into the COLL/HA matrix and thus, the release will have two individual mechanisms of release, a diffusional one from the matrix (faster) and one from the mesoporous system [3].

The obtained materials were characterized from morphological and structural point of view by specific techniques: Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), Ultraviolet-Visible Spectra Measurement (UV-Vis), Photoluminescence spectra (PL) and Thermogravimetric Analysis (TGA). The in vitro study was performed in simulated biological fluids. Finally, the obtained materials will be tested for various biomedical applications as systems with controlled release of polyphenols extracted from natural sources, including tissue engineering with a focus on regeneration and antimicrobial activity.

Acknowledgement: The authors are acknowledging the support of the project 29ROMD/20.05.2024: "Nanostructured bone grafts with predetermined properties" and to the Romanian Government for providing access to the research infrastructure of the National Centre for Micro and Nanomaterials through the National Program titled "Installations and Strategic Objectives of National Interest".

References: **[1]** Petrisor, G., et al., Increasing Bioavailability of Trans-Ferulic Acid by Encapsulation in Functionalized Mesoporous Silica. Pharmaceutics, 2023. 15(2).; **[2]** Jian M. et al. Caracterizarea structurilor tridimensionale din colagen extras din complexul ombilico-placentar pentru aplicații în chirurgia oro-maxilo-facială //Intellectus. – 2024. – №. 1. – С. 179-188; **[3]** Anton Ficai, Ecaterina Andronescu, Georgeta Voicu, Cristina Ghitulica, Bogdan Stefan Vasile, Denisa Ficai, Viorica Trandafir; Self assembled collagen/hydroxyapatite composite materials; Chemical Engineering Journal, 2010;160(2), 1385-8947

SC-P08 *IN VITRO* BIOLOGICAL STUDIES OF SOME HYDROGELS FUNCTIONALIZED WITH DIHYDROPYRIMIDINE DERIVATES

Claudia Valentina Popa[1,2*], Razvan Neagu[1], Lucia-Elena Ionescu[1], Radu-Iulian Tanasa[1], Diana-Mihaela Popescu[1], Cristina-Anca Secara[1], Maria Marinescu[2*]

[1]"Cantacuzino" National Military Medical Institute for Research and Development, 103 Splaiul Independenței, 050096, Bucharest, Romania
[2] University of Bucharest, 90 Sos. Panduri, 050663, Bucharest, Romania

Abstract: *In vitro biological activities of some obtained hydrogels functionalized with dihydropyrimidine derivates were determined.*
Key words: hydrogel; dihydropyrimidine derivates; antibacterial; antiviral

Introduction: The properties of hydrogels mimic the natural extracellular matrix, supporting wound regeneration [1]. DHPM derivatives have many biological properties, such as: antitumour, antiviral and antimicrobial activities [2]. The main objective of this study is to determine the antibacterial and antiviral activities of Carbopol-based hydrogels functionalized with some DHPMs.

Experimental and/or Modelling: Ethyl 4-(2-R-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate derivatives, where R is (**1**) 3-OH; (**2**) 4-Cl; (**3**) 2-naphthyl, were synthetized through on Biginelli condensation and its structures were confirmed by NMR spectra. Functionalized carbopol-based hydrogels were obtained. Standard reference strains of *S. aureus*, *E. coli* and *P. aeruginosa* were used in antimicrobial activity determination. The MTT assay based on L-929 mouse fibroblasts was applied for the cytotoxicity evaluation of hydrogels. Antiviral activity screening was performed on HeLa cell lines.

Results and discussions: The functionalized hydrogels showed good antibacterial and antiviral activities and were negative in terms of cytotoxicity.

Conclusions: The antimicrobial and antiviral activities of hydrogels functionalized with DHPMs were good. *In vivo* studies are required.

References:

[1] Thi K.N.D., Thi T.T., Thi N.L.P., Thi X.N., Vu H.M.D., Truong T.V., Jaeyeop C., Umapada P., Prodyut D., Byeongil L., Junghwan O., Sudip M., Hydrogel-Based Smart Materials for Wound Healing and Sensing, *Aggregate*, 6, 6 (2025), e 70047.

[2] Marinescu M., Popa C.V., Pyridine Compounds with Antimicrobial and Antiviral Activities, *Int J Mol Sci*., 23(2022), 5659.

Acknowledgements: This work was supported by the SRDP project of the Ministry of National Defense „Innovative pharmaceutical preparations with topical administration and antimicrobial activity based on new synthetic hybrid compounds"

* Corresponding authors: popa.claudia @cantacuzino.ro; maria.marinescu@chimie.unibuc.ro

SC-P09 CHARACTERIZATION OF THE THERMO-HYGROMETRIC BEHAVIOR OF NATURAL WOOL AND EXPANDED POLYSTYRENE INSULATION MATERIALS IN BUILDING APPLICATIONS

[1]A.M. Asoltanei*, [1]E.T. Iacob - Tudose, [1]M.S. Secula, [1]E.N. Dragoi, [2]D.N. Isopescu and [1]I. Mamaliga

[1]Gheorghe Asachi Technical University of Iasi, Faculty of Chemical Engineering and Environmental Protection, 73 D. Mangeron Street, 700050, Iasi, Romania

[2]Gheorghe Asachi" Technical University of Iasi Faculty of Civil Engineering and Building Services, 1 Prof. D. Mangeron Blvd., 700050 Iași, Romania

Abstract: *This study presents a comparative analysis of the thermo-hygrometric behavior of natural wool and expanded polystyrene (EPS) insulation materials. It is based on an analytical model describing the kinetics of water vapor absorption in a planar layer of thickness L. The normalized absorption rate Mt/M is mathematically expressed using the effective diffusion coefficient D_{eff}, revealing considerable differences in vapor permeability between the materials. The methodology integrates experimental determinations, thermal cycling, and numerical heat-air-moisture (HAM) simulations for rigorous validation of thermo-hygrometric performance and durability. The results highlight the superior moisture buffering capacity and climatic resilience of natural wool and recommend hybrid system integration to enhance sustainable thermal insulation.*

Keywords: vapor diffusion, natural wool, expanded polystyrene, heat-air-moisture modeling, moisture buffering value (MBV)

Introduction: Effective moisture management and optimization of thermo-hygrometric properties are critical to building envelope durability and energy performance. Insulation materials must exhibit low thermal conductivity along with sufficient vapor permeability to minimize condensation and structural damage risks. Natural wool and expanded polystyrene constitute two fundamentally different materials with distinct microstructural and chemical traits influencing vapor diffusion.

Experimental and/or Modelling: An established analytical expression describing the vapor absorption rate in planar materials is used:

$$\frac{M_t}{M} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp\left(-\frac{(2n+1)^2 \pi^2 D_{\text{eff}} t}{4L^2}\right),$$

where M_t and M are vapor masses at time t and equilibrium, respectively; D_{eff} is the effective vapor diffusion coefficient. All coefficients were experimentally determined via gravimetric sorption methods, supplemented by thermal conductivity measures and cyclic hygrothermal exposure. Findings were corroborated through comprehensive heat-air-moisture (HAM) simulations under realistic environmental conditions.

* Corresponding author: adriana-mariana.asoltanei@student.tuiasi.ro

Results and discussions: Natural wool exhibited an effective diffusion coefficient D_{eff} of the order of $6x10^{-8}$ m^2/s, significantly higher than EPS, which ranged between 10^{-11} and 10^{-12} m^2/s. This disparity accounts for wool's substantially enhanced moisture buffering capacity, as corroborated by its markedly higher Moisture Buffering Value metrics. Wool displayed remarkable retention of thermal insulation and structural integrity after over 100 hygrothermal cycles, whereas EPS showed early onset of material degradation including microcracking and increased thermal conductivity. Numerical simulations confirmed that hybrid insulation configurations effectively mitigate condensation risk effectively.

Conclusions: The integration of analytical vapor sorption models with experimental data validates natural wool as a highly durable and sustainable thermo-hygrometric insulation material. Strategic hybridization with EPS optimizes overall system performance for contemporary sustainable building envelopes.

SC-P10 ECO-FRIENDLY BIO-CATALYSTS FROM FISH WASTE FOR DYE REMOVAL IN WATER TREATMENT

Raluca Florenta Doroftei [1], Mihaela Silion [2], Daniela Ioniță [2], Andrei Dascalu [2], Florin Nedeff [3], Ana-Maria Georgescu [4], Ana-Maria Rosu [4], Diana Mirila [3,*] and Ileana-Denisa Nistor [4]

[1] School of Doctoral Studies, "Vasile Alecsandri" University of Bacau, 157 Calea Marasesti Street, 600115 Bacau, Romania;

[2] Physics of Polymers and Polymeric Materials, "Petru Poni" Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487 Iasi, Romania;

[3] Department of Environmental Engineering, Mechanical Engineering and Agritourism, Faculty of Engineering, "Vasile Alecsandri" University of Bacau, 157 Calea Marasesti Street, 600115 Bacau, Romania;

[4] Department of Chemical and Food Engineering, Faculty of Engineering, "Vasile Alecsandri" University of Bacau, 157 Calea Marasesti Street, 600115 Bacau, Romania;

Abstract: *The widespread use of synthetic dyes such as Malachite Green (MG) in aquaculture and industry has led to persistent contamination of water bodies, raising concerns about ecological toxicity and human health risks. This study proposes an innovative and sustainable approach to MG removal by valorizing fish processing waste, specifically scales and swim bladders from Cyprinus carpio, as multifunctional biomaterials for both adsorption and catalytic ozonation.*

Raw and vanadium-functionalized biomaterials were synthesized and thoroughly investigated using advanced structural, morphological, thermal, and molecular characterization techniques to assess their adsorption and catalytic properties. Adsorption experiments revealed that fish scales exhibited superior performance, achieving over 90% dye removal, while fish bladder reached over 80% under optimized conditions. Upon vanadium impregnation, FS-V demonstrated enhanced catalytic activity, achieving over 63 % MG degradation at low ozone flow rates (0.5 g $O_3 \cdot h^{-1}$*), outperforming FB-V across all tested parameters [1].*

The dual functionality of these biomaterials, adsorptive retention and oxidative degradation, offers a promising alternative to conventional treatment methods. This research highlights the role of vanadium in promoting reactive oxygen species generation and improving surface reactivity, particularly in FS-V, which showed higher vanadium incorporation and structural uniformity. pH evolution and degradation kinetics further confirmed the catalytic efficiency and stability of the materials.

By integrating waste valorization with advanced oxidation processes, this research contributes to circular economy principles and opens new avenues for low-cost, scalable water purification technologies. The findings underscore the potential of fish-derived bio-catalysts in mitigating dye pollution and support their application in wastewater treatment systems.

Keywords: bioadsorbents; catalytic ozonation; vanadium; fish waste valorization; environmental remediation.

Reference

1. Doroftei, R.F.; Silion, M.; Ioniță, D.; Dascalu, A.; Nedeff, F.; Georgescu, A.-M.; Rosu, A.-M.; Mirila, D.; Nistor, I.-D. From Nature to Remediation: Biomaterials for Malachite Green Retention and Degradation. *Materials* **2025**, *18*, 4374.

* Corresponding author: miriladiana@ub.ro

SC-P11 GELATIN-CLAY HYBRID COMPOSITES FOR DYE ADSORPTION IN FOOD INDUSTRY APPLICATIONS

Ana-Maria Georgescu[1], Ana-Maria Rosu [1*], Gabriela Muntianu[1], Emilian Mosnegutu[2], Diana Mirila[2], and Ileana-Denisa Nistor [1]

[1] Department of Chemical and Food Engineering, Faculty of Engineering, "Vasile Alecsandri" University of Bacau, 157 Calea Marasesti Street, 600115 Bacau, Romania;

[2] Department of Environmental Engineering, Mechanical Engineering and Agritourism, Faculty of Engineering, "Vasile Alecsandri" University of Bacau, 157 Calea Marasesti Street, 600115 Bacau, Romania

Abstract: *Synthetic dyes are widely used in the food industry to enhance product appeal, but their persistence and potential toxicity raise concerns regarding food safety and environmental impact. As the demand for natural alternatives increases, the development of efficient materials for dye stabilization and removal becomes essential. Organo-inorganic hybrid matrices, such as gelatin-clay composites, offer promising features due to their structural adaptability and functional properties. This research investigates the potential of a gelatin-montmorillonite K10 hybrid matrix for the adsorption of representative synthetic food dyes.*

Gelatin-montmorillonite composites combine the biocompatibility and film-forming ability of gelatin with the high surface area, layered structure, and ion-exchange capacity of montmorillonite clay. Gelatin, a natural biopolymer derived from collagen, offers functional groups such as amino and carboxyl groups that facilitate interactions with various chemical species. Montmorillonite, a smectite-type clay, contributes to the mechanical stability and adsorption capacity of the hybrid material due to its expandable interlayer spaces and negatively charged surfaces. The synergistic integration of these components results in a versatile matrix capable of interacting with a wide range of organic molecules.

Characterization techniques including Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy (SEM-EDX), Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and UV-Vis spectrophotometry were employed to evaluate the material before and after dye exposure. SEM-EDX provided insights into surface morphology and elemental composition, FTIR analysis suggested possible interactions between functional groups of the matrix and dye molecules, while XRD revealed structural changes in the clay component. Preliminary UV-Vis results indicate promising adsorption capacities, particularly for certain cationic dyes.

These findings highlight the potential of gelatin-clay composites as promising adsorbents for synthetic dyes, with applications in environmental remediation. Further research will focus on optimizing synthesis parameters and expanding the range of target contaminants.

Keywords: gelatin, K10 clay, adsorption, food dyes, hybrid materials, wastewater treatment.

[*] Corresponding author: ana.rosu@ub.ro

SC-P12 OPERATION OF A LARGE WASTEWATER TREATMENT PLANTS FOR BIOGAS PRODUCTION

Claudia Ana Maria CANTARAGIU [1]*, Doinița-Roxana TÎRPAN[2] and AnaMaria NICULESCU ILIE[1,2]

[1] University Politehnica of Bucharest, Chemical and Biochemical Engineering Department, 1-6 Gheorghe Polizu, 011061, Bucharest, Romania

[2] Ovidius University of Constanta, Chemistry and Chemical Engineering Department, 124 Mamaia Blvd., 900527, Constanta, Romania

Abstract: *In this study, biogas was obtained using sludge from wastewater treatment plant.*
Key words: Anaerobic fermentation, Wastewater treatment, Biogas

Introduction: Anaerobic fermentation in the world is seen as a very beneficial solution from two points of view: solving the problem of waste and energy production. Wastewater treatment is a process used to remove contaminants from wastewater or sewage and convert it into an effluent that can be returned to the water cycle with minimum impact on the environment or directly reused. The plants contain many phases of hydrodynamic processing of heterogeneous systems.
Experimental: The experimental part of this study concerns the commissioning of a biogas fermenter and the long-term tracking of the operation of the biogas line coupled with the electric cogeneration line and hot water for the process. On average, at a fermentation station, approximately 400–600 m^3 of biogas can be obtained from a tone of waste mixture, of which 50–70% can be methane.
Results and discussions: Throughout the start-up of the digester, the flow to be supplied, the total solid concentration at the entry and exit into and out of the bioreactor, the total volatile concentration (fermentable) at the entry and exit of the fermenter and the gas flow produced by the fermenter has been measured. The monitoring period of the parameters was 70 days. Anaerobic fermentation results in a biogas in which the carbon dioxide content does not exceed 38% vol. The summary shows that from 1900 m^3/day sludge fed in digesters produces 24000 m^3/day of biogas. The cogeneration station powered by two 1000 m^3 gasometers operates with two 2 MWh gas engines each, which produce electricity and heat.
Conclusions: The results obtained allow for the continuation and development of other directions within the same topic.
References:

1. Rapport J., Zhang R., Jenkins M. B., Williams B R., *Current Anaerobic Digestion Technologies Used for Treatment of Municipal Organic Solid Waste, Biomass and Bioenergy*., 35, 3, 1263 - 1272, 2011

* Corresponding author: patrichi.claudia@gmail.com

SC-P13 NEXT-GENERATION MESOPOROUS MCM-41 PLATFORMS FOR VITAMIN C ENCAPSULATION: BRIDGING MATERIAL INNOVATION AND PHARMACEUTICAL EFFICACY

Bogdan Purcăreanu[1,2], Mihai Alexandru Florea[2,*], Manuela Diana Ene[2], Sabina Cristiana Bădulescu[2,3], Dan Eduard Mihaiescu[4], Mihai Alexandru Grigoroscuta[5], Petre Badica[5], Anton Ficai[1,6]

[1]Department of Science and Engineering of Oxide Materials and Nanomaterials, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, Gh. Polizu 1-7, 011061, Bucharest, Romania

[2]Biotehnos SA, Gorunului Street 3-5, 075100, Otopeni, Romania

[3]Faculty of Pharmacy, "Carol Davila" University of Medicine and Pharmacy, Traian Vuia 6, 020956, Bucharest, Romania

[4]Department of Organic Chemistry "Costin Neniţescu", Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, Gh. Polizu 1-7, 011061, Bucharest, Romania

[5]National Institute of Materials Physics, Street Atomistilor 405 A, 077125 Magurele, Romania

[6]Academy of Romanian Scientists, 3 Ilfov St., 050045 Bucharest, Romania

Abstract: *Over the past decades, since their discovery, mesoporous materials have attracted considerable scientific attention due to their unique structural and physicochemical properties. Among them, MCM-41 stands out as one of the most versatile and promising carriers for controlled drug delivery, owing to its high surface area, ordered pore structure, and remarkable loading capacity for active pharmaceutical ingredients. Ascorbic acid (vitamin C), a water-soluble antioxidant essential for immune function and protection against oxidative stress, represents a compound whose stability and controlled release remain major challenges in pharmaceutical formulations. In this study, vitamin C was encapsulated within the pores of MCM-41 materials functionalized with different surface groups (–OH, –COOH, –NH_2, and –CH_3) to enhance its stability and achieve sustained release profiles. The synthesized materials were thoroughly characterized using SEM, DLS, FT-IR, and BET analyses, while the vitamin C-loaded samples were further examined by FT-IR and BET to confirm successful encapsulation. The qualitative monitoring of vitamin C desorption was conducted by UV–VIS spectrophotometry, allowing the evaluation of its release behavior over time. Experimental findings demonstrated that the MCM-41 material functionalized with amino (–NH_2) groups exhibited superior protective effects on vitamin C, ensuring enhanced stability and a prolonged release exceeding 12 hours. These results highlight the potential of surface-engineered mesoporous silica as an advanced platform for the development of efficient and stable pharmaceutical delivery systems for sensitive bioactive compounds.*

Key words: mesoporous material, MCM-41, functionalization, vitamin C, controlled release

Acknowledgments: This work has been funded by the Romanian National Authority for Scientific Research and Innovation, CNCS UEFISCDI, project no. PN-IV-P7-7.1-PED-2024-2569, 63PED/08.01.2025 (SYSDELBIO).

* Corresponding author: alexandru.florea@biotehnos.com

References:

[1] Kurbonov, S.; Czigány, Z.; Kovács, Z.; Péter, L.; Pisárˇcik, M.; Lukáˇc, M.; Kriechbaum, M.; Ryukhtin, V.; Lacrămă, A.-M.; Almásy, L. Structural Characterization of Ordered Mesoporous Silica Prepared by a Sol–Gel Process Using Urea Based Cationic Gemini Surfactants. *Gels* (2025), 11, 804. https://doi.org/10.3390/gels11100804;

[2] Karczmarska, A.; Laskowska, W.; Stró ˙z, D.; Pawlik, K. Inside the Framework: Structural Exploration of Mesoporous Silicas MCM-41, SBA-15, and SBA-16. *Materials* (2025), 18, 3597. https://doi.org/10.3390/ma18153597;

[3] Kim,W.;Lee,K.;Kim,H.; Choi, M.;Hong,S.-K.;Lee,J.E. RemovalofMetalIonsinSpin-on HardmaskUsingFunctionalized PorousSilica Adsorbents. *Appl. Sci*. (2025), 15, 7185. https://doi.org/10.3390/app15137185;

[4] Sibao Zhao, Wenzhen Qiu, Yang Sun, Feng Jin, Fengjun Wang, Development and characterization of a walnut protein hydrolysate-Fe-vitamin C complex: Enhancing iron bioavailability through phytase-assisted modification. *Food Chemistry*, Volume 496, Part 1, 25 December 2025, 146646, https://doi.org/10.1016/j.foodchem.2025.146646.

SC-P14 IN VITRO TESTING OF CONTROLLED-RELEASE VITAMIN C FORMULAE FOR MODULATION OF IMPORTANT THERAPEUTIC EFFECTS IN SKIN REPAIRING

Sabina Cristiana Badulescu[1,2*], Manuela Diana Ene[2], Bogdan Purcareanu[2,3], Alexandru Mihai Florea[2], Andrei Kuncser[4], Petre Badica[4], Rica Boscencu[1]

[1] Faculty of Pharmacy, "Carol Davila" University of Medicine and Pharmacy, Traian Vuia 6, 020956, Bucharest, Romania
[2] Biotehnos SA, Gorunului Street 3-5, 075100, Otopeni, Romania
[3]Department of Science and Engineering of Oxide Materials and Nanomaterials, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, Gh. Polizu 1-7, 011061
[4] National Institute of Materials Physics, Atomistilor street 405A, 077125 Magurele

Abstract:
Vitamin C is an old-age recognized remedy (18th century treatment for scurvy; 19th century chemical isolation)[1], and it has been largely promoted in the last decades for its antioxidant, collagen-boosting, brightening, whitening, anti-aging, moisturizing, reducing acne and wound healing properties in relation to the skin [2,3]. Vitamin C is sensitive to environmental factors such as heat, light – UV rays, water, high pH, oxygen, metal ions [4,5,6]. These factors speed up its degradation or transformation into completely useless products for human health, thus making the processing of this compound into a medicine or a cosmetic formulation, a challenge.
Mesoporous materials, such as MCM-41, are biocompatible silica matrices. MCM-41 is used for drug release due to its high surface area, high pore volume and ordered hexagonal mesoporous structure. Nonetheless, surface chemical modification can be achieved by grafting functional groups: amino-, phenyl-, chloro-, carboxy-, methyl- and so on. This allows changes in particle morphology and non-cytotoxic nature. The modified surface is convenient to achieve a better compatibility with hydrophilic or hydrophobic ingredients [7,8,9,10].
In particular, surface grafting of MCM-41 can increase the strength of the physicochemical interactions between vitamin C and the silica matrix, allowing for the design of desired release profiles. This strategy offers the possibility to identify the optimal concentration of the active ingredient (API), alone and in combination with other anti-oxidants - to achieve therapeutic efficacy, a good control of the its release and also its protection against degradation.
We tested several formulations of amino-functionalized MCM-41 loaded with vitamin C and combined with ferulic acid and / or oryzanol (ferulic acid esters extracted from rice bran), known for their anti-oxidant and anti-inflammatory effects, on the human dermal fibroblast cell line HS27. In the context of wound healing and skin health, we aimed to observe tissue regeneration by cell migration into a wound site using real time microscopic monitorization by scratch test. In order to determine the optimal formulation in terms of vitamin C stability, sustained-release and therapeutic efficacy, we quantified collagen production and degradation, cellular proliferation, oxidative protection and interleukin modulation.

Acknowledgments:

Authors acknowledge UEFISCDI for support through project PED 63/2025, SYSDELBIO.

* Corresponding author: Email address: sabina.serbu@biotehnos.com

References:

[1] Luft, E., *Lind Discovers a Cure for Scurvy*. EBSCO Information Services Inc., 2023. Available from: https://www.ebsco.com/research-starters/history/lind-discovers-cure-scurvy

[2] Wang, K., Jiang, H., Li, W., Qiang, M., Dong, T., & Li, H. (2018). Role of vitamin C in skin diseases. *Frontiers in Physiology*, *9*(JUL). https://doi.org/10.3389/fphys.2018.00819

[3] Pullar, J. M., Carr A. C., Vissers, M. C. M., The roles of vitamin C in skin health, *Nutrients*, 9, 8, (2017).

[4] Alberts, A., Moldoveanu, E. T., Niculescu, A. G., & Grumezescu, A. M., Vitamin C: A Comprehensive Review of Its Role in Health, Disease Prevention, and Therapeutic Potential. *Molecules*, 30, 3, (2025).

[5] Carr A.C., Maggini, S., Vitamin C and immune function, *Nutrients*, *9*, 11, (2017).

[6] Giannakourou, M. C., & Taoukis, P. S., Effect of alternative preservation steps and storage on vitamin c stability in fruit and vegetable products: Critical review and kinetic modelling approaches. *Foods*, 10, 11, (2021).

[7] Horcajada P., Rámila A., Férey G., Vallet-Regí M., Influence of superficial organic modification of MCM-41 matrices on drug delivery rate, *Solid State Sciences*, 8, 10, (2006), 1243-1249.

[8] Manzano, M., Aina, V., Areán, C. O., Balas, F., Cauda, V., Colilla, M., Delgado, M. R., Vallet-Regí, M., Studies on MCM-41 mesoporous silica for drug delivery: Effect of particle morphology and amine functionalization. *Chemical Engineering Journal*, *137*(1), (2008), 30–37.

[9] Cuello N.I., Elías V. R., Mendieta S.N., Longhi M., Crivello M. E., Oliva M.I., Eimer G.A., Drug release profiles of modified MCM-41 with superparamagnetic behavior correlated with the employed synthesis method, *Materials Science and Engineering: C*, 78, (2017), 674-681.

[10] Pandele A.M., Andronescu C., Ghebaur, A., Garea S.A., Iovu, H., New biocompatible mesoporous silica/polysaccharide hybrid materials as possible drug delivery systems. *Materials*, 12, 1, (2018).

SC-P15 ADVANCED MXENE–POLYMER NANOCOMPOSITES AS SOFT MATERIALS FOR EMI SHIELDING, LIGHT-DRIVEN ACTUATION, AND BIOMEDICAL APPLICATIONS

Gabriela Toader [1], Aurel Diacon [1, *], Alexandra Mocanu [2], Livia A. Dinu [2], Pericle Varasteanu [2], Oana Brincoveanu [2], Cosmin Romanitan [2], Mioara Alexandru [3], Florina L. Zorila [3], Celina Damian [4], Edina Rusen [4], Raul A. Mitran [5]

[1]Military Technical Academy "Ferdinand I", 39-49 G. Cosbuc Blvd., 050141 Bucharest, Romania

[2] National Institute for Research and Development in Microtechnologies - IMT Bucharest, 126A Erou Iancu Nicolae, 077190 Voluntari, Romania.

[3] Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (NIPNE), 30 Reactorului St., 077125 Magurele, Romania

[4] Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology POLITEHNICA Bucharest, 1-7 Gheorghe Polizu St., 1st District, 011061 Bucharest, Romania

[5] "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 Splaiul Independentei, Bucharest, 060021, Romania

Abstract: *A novel class of MXene–polymer nanocomposites has been developed, integrating pristine MXenes such as Nb_2AlC, $Mo_2Ti_2AlC_3$, and Ti_3AlCN into various polymer matrices, including polyurethane foams and films, epoxy resins, and hydrogels. These composites exhibit enhanced electromagnetic interference (EMI) shielding, mechanical flexibility, actuation capabilities, and biocompatibility. Sustainable synthesis techniques and targeted chemical functionalization were employed to optimize performance across electronic, biomedical, and soft robotic applications.*
Key words: responsive hydrogel, MXenes, polypyrrole, biomedical applications, actuation.

Introduction: MXenes, a family of two-dimensional transition-metal carbides and nitrides, have attracted significant attention for their high electrical conductivity, hydrophilicity, and tunable surface chemistry [1]. Their layered morphology and aspect ratio make them ideal candidates for polymer integration, enabling multifunctional properties such as mechanical reinforcement and stimulus responsiveness [2-4]. This study explores the synthesis and application of MXene–polymer nanocomposites tailored for EMI shielding, actuation, and biomedical use. Sustainable approaches and functionalization strategies were employed to enhance compatibility and performance.

Experimental: *Reagents:* Pristine MXenes (Nb_2AlC, $Mo_2Ti_2AlC_3$, Ti_3AlCN) were used alongside polymers, including recycled poly(ethylene terephthalate), epoxy resins, and poly(N-isopropylacrylamide). *Preparation of composites*: PUR foams were synthesized via PET depolymerization, while PUR films incorporated

* Corresponding author:

$Mo_2Ti_2AlC_3$ MXenes. Epoxy nanocomposites were fabricated using soap-free emulsion polymerization. *Functionalization and encapsulation*: MXenes were chemically modified with –SH, $–NH_2$, and –OH/oxyrane groups after HF etching. Microencapsulation using poly(methyl methacrylate-co-hydroxypropyl methacrylate) stabilized MXene dispersion. *Hydrogel integration:* $Mo_2Ti_2AlC_3$ and Ti_3AlCN MXenes were embedded into PPy and pNiPAM-based hydrogels, respectively, enabling responsive behavior under thermal and NIR stimuli.

Results and discussions: The performance of MXene–polymer nanocomposites was evaluated. Samples containing Nb_2AlC incorporated into recycled PUR foams demonstrated high electromagnetic interference (EMI) attenuation due to their porous structure and conductivity. $Mo_2Ti_2AlC_3$-enhanced polyurethane films exhibited improved mechanical resilience and shielding capabilities. Microcapsule-stabilized MXenes maintained structural integrity under stress conditions. Epoxy composites demonstrated tunable electromagnetic properties that varied with colloid concentration. Hydrogels incorporating $Mo_2Ti_2AlC_3$ and polypyrrole displayed low swelling and high conductivity, making them suitable for wearable electronics. Additionally, Ti_3AlCN included in pNiPAM hydrogels facilitated reversible actuation. Functionalized MXenes enhanced dispersion and biocompatibility. Silver-decorated SH-MXene hydrogels achieved up to a 5-log reduction in bacterial count against Staphylococcus aureus, confirming their antimicrobial efficacy.

Conclusions: MXene–polymer nanocomposites present a versatile platform for various multifunctional applications, including EMI shielding, soft robotics, and biomedicine. Through sustainable synthesis, filler stabilization, and chemical functionalization, these materials demonstrate tunable electrical, mechanical, and biological properties. Consequently, MXenes play a crucial role in advancing next-generation smart materials.

Acknowledgments*: This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CNCS UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0466 - ctr. no. 2PTE/2025, project number PN-IV-P7-7.1-PED2024-0980 ctr. no. 69PED/2025, and project number PN-IV-P7-7.1-PTE-2024-0479 – ctr.no. 42PTE/2025.*

References:

[1]. B. Anasori, J. Halim, J. Lu, C. A. Voigt, L. Hultman, and M. W. Barsoum, - Mo2TiAlC2: A new ordered layered ternary carbide, *Scripta Materialia*, 101, (2014), 5-7.

[2]. Y. Vasseghian, E.-N. Dragoi, F. Almomani, and V. T. Le, - A comprehensive review on MXenes as new nanomaterials for degradation of hazardous pollutants: Deployment as heterogeneous sonocatalysis, *Chemosphere,* 287, 2021, 132387.

[3]. H. Yang, G.-X. Zhang, H.-J. Zhou, Y.-Y. Sun, and H. Pang, - Metal–Organic Frameworks Meet MXene: New Opportunities for Electrochemical Application, *Energy Material Advances*, 4, (2023), 33.

[4]. P. Panigrahi, Y. Pal, T. Kaewmaraya, H. Bae, N. Nasiri, and T. Hussain, - Molybdenum Carbide MXenes as Efficient Nanosensors toward Selected Chemical Warfare Agents, *ACS Applied Nano Materials*, 6 (10), (2023), 8404-8415.

SC-P16 MXENE–POLYPYRROLE-HYDROGELS AS VERSATILE SOFT MATERIALS FOR EMI SHIELDING

Andreea Moldovan[1], Aurel Diacon [1,*], Gabriela Toader [1], Martino Aldrigo [2], Sergiu Iordănescu [2], Alexandra Mocanu [2], Oana Brincoveanu [2], Cosmin Romanitan [2], Traian Rotariu [1], Edina Rusen [3], Ana Mihaela Gavrila 4, Bodan Trica[5]

[1]Military Technical Academy "Ferdinand I", 39-49 G. Cosbuc Blvd., 050141 Bucharest, Romania

[2] National Institute for Research and Development in Microtechnologies - IMT Bucharest, 126A Erou Iancu Nicolae, 077190 Voluntari, Romania.

[3] Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology POLITEHNICA Bucharest, 1-7 Gheorghe Polizu St., 1st District, 011061 Bucharest, Romania

[4] National Research and Development Institute for Chemistry and Petrochemistry ICECHIM, Advanced Polymer Materials and Polymer Recycling, 202 Splaiul Independentei, 060021 Bucharest, Romania

Abstract: *Semi-interpenetrated polymer network (sIPN) hydrogels incorporating Mo_2TiAlC_3 MXenes and polypyrrole (PPy) were synthesized via photopolymerization. These composites exhibited reduced swelling, enhanced mechanical strength, and effective EMI shielding in the X-band. The optimized formulation (0.1 wt.% MXene) demonstrated superior conductivity and absorption-dominated shielding, highlighting its potential for EMI shielding or flexible electronics.*
Key words: MXene hydrogels, EMI shielding, polypyrrole, soft electronics.

Introduction: Composites are a very important class of engineering materials. Today, there is an urgent need for lightweight, flexible EMI shielding materials. Traditional metal-based shields are limited by their rigidity and susceptibility to corrosion. MXenes, especially Mo_2TiAlC_3, offer high conductivity and tunable surface chemistry [1,2]. Hydrogels provide a versatile matrix for integrating MXenes and conductive fillers. This study presents the synthesis and characterization of Mo_2TiAlC_3–PPy hydrogels for EMI shielding applications.
Experimental: *Reagents:* HEMA, AA, PVA, Mo_2TiAlC_3 MXenes, and PPy particles. *Hydrogel synthesis:* Photopolymerization of HEMA and AA in PVA formed sIPN hydrogels. MXenes were ultrasonicated in PVA for dispersion. PPy was synthesized and co-incorporated. *Characterization:* Samples with 0.1–0.4 wt.% MXenes were analyzed via SEM, TEM, FT-IR, TGA, XRD, mechanical testing, and EMI shielding in the X-band (8.2–12.4 GHz).
Results and discussions: Hydrogels showed >98% gel fraction, confirming strong crosslinking. The addition of MXene reduced swelling and improved network density. SEM and TEM revealed uniform filler dispersion, and pore sizes decreased with increasing MXene content. FT-IR and XRD confirmed successful incorporation and partial exfoliation. TGA showed enhanced thermal stability. Mechanical tests indicated improved strength at 0.1–0.2 wt.% MXenes; higher loading caused agglomeration. EMI tests showed the highest shielding at 0.1 wt.%

due to optimal conductivity and filler distribution. PPy enhanced absorption-dominated shielding, reducing reflection losses.

Conclusions: Mo_2TiAlC_3 MXenes and PPy were successfully integrated into sIPN hydrogels. The resulting composites exhibited low swelling, improved mechanical properties, and effective EMI shielding. These materials are promising for flexible electronics and biomedical applications.

Acknowledgments*: This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CNCS UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0466 - ctr. no. 2PTE/2025, project number PN-IV-P7-7.1-PTE-2024-0517– ctr.no. 15PTE/2025.*

References:

[1]. B. Anasori, J. Halim, J. Lu, C. A. Voigt, L. Hultman, and M. W. Barsoum, - Mo2TiAlC2: A new ordered layered ternary carbide, *Scripta Materialia*, 101, (2014), 5-7.

[2]. H. Yang, G.-X. Zhang, H.-J. Zhou, Y.-Y. Sun, and H. Pang, - Metal–Organic Frameworks Meet MXene: New Opportunities for Electrochemical Application, *Energy Material Advances*, 4, (2023), 33.

BOOK OF ABSTRACTS

SICHEM – 2025

D – Green applied chemistry and agro-resources valorization (GACARV)

1. Oral presentations

SD-OP01 VALORIZATION OF LIVESTOCK AND POULTRY MANURE THROUGH BIOCHAR PRODUCTION AND ITS AGRICULTURAL APPLICATIONS

Zhonghua Cui[1,2*], Alexandru Ozunu[2], Jun Meng[1]

[1] Institute of Eco-environmental Research, School of Environmental and Natural Resources, Zhejiang University of Science & Technology, Hangzhou 310023, China

[2] Babeş-Bolyai University of Cluj-Napoca, Faculty of Environmental Science and Engineering, Doctoral School of Environmental Science - 30 Fantanele Street, RO-400294, Cluj-Napoca, Romania.

Abstract: *Livestock and poultry manure is an abundant by-product of intensive farming, but its improper disposal often leads to nutrient loss and environmental pollution. Converting manure into biochar through thermal treatment provides an effective green-chemistry pathway for resource valorization. In this study, manure-derived biochars were prepared by slow pyrolysis at different temperatures (300-700 °C), and their physicochemical characteristics and agricultural benefits were evaluated. Results showed that pyrolysis temperature strongly affected biochar pH, ash content, and specific surface area. Higher temperatures increased carbon stability but reduced nitrogen content, while moderate temperatures (400-500 °C) produced biochar with balanced nutrient retention and surface functionality. When applied to acidic soils, manure biochar significantly increased soil pH, cation exchange capacity (CEC), and available phosphorus, leading to better plant growth and yield compared with untreated soil. Moreover, biochar application reduced the mobility of heavy metals and enhanced soil carbon sequestration potential. Overall, manure-derived biochar represents a sustainable strategy for nutrient recycling, soil improvement, and waste reduction in agriculture. Future work should optimize pyrolysis conditions and field application rates to achieve stable agronomic performance and minimize potential risks.*

Keywords: Manure; Biochar; Pyrolysis, Soil Fertility, Nutrient Recycling, Sustainable Agriculture

* Corresponding author: zhonghua.cui@ubbcluj.ro

SD-OP02 PYROLYSIS OF PLASTIC WASTE TO OBTAIN GASEOUS FUEL

Pșenovschi Grigore[1,2*], Ioan Călinescu[1], Ciprian-Gabriel Chisega-Negrilă[1], Cristina-Emanuela Enășcuță[2]

[1]NUST POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, 1-7 Gheorghe Polizu St., 011061, 1st district, Bucharest, Romania

[2]INCDCP-ICECHIM Bucharest, 202 Spl. Independentei, 6 th district, Romania

Abstract: *This study investigates microwave-assisted pyrolysis as a sustainable approach for valorizing polypropylene (PP) and polyethylene (PE) waste, emphasizing the enhancement of gaseous product formation, particularly hydrogen-rich components. The experiments were performed in a monomode microwave reactor, where the polymer feedstock was layered with silicon carbide, serving as a microwave susceptor, and activated carbon acting as a catalyst. The research systematically evaluated the influence of catalyst loading, reactor configuration, and polymer type. For all tested materials, the resulting gases exhibited high heating values (46,941–55,087 kJ/kg) and low specific CO_2 emissions (4.4–6.1 × 10^{-5} kg CO_2/kJ), reflecting both strong energetic potential and a diminished carbon impact. Overall, the results demonstrate that microwave-assisted pyrolysis represents an efficient route for converting end-of-life vehicle (ELV)-derived plastic waste into valuable energy carriers.*

Keywords: activated carbon, microwave-assisted pyrolysis, waste, waste-to-energy, susceptor, hydrogen

Introduction: Plastic waste has become a pressing issue in Romania, driven by the continuous growth in volumes from industrial sources, particularly end-of-life vehicles (ELVs), and by the urgent need to mitigate environmental impacts [1, 2]. Conventional recycling methods remain limited for mixed or contaminated plastics, prompting interest in thermochemical conversion routes such as pyrolysis. Among these, microwave-assisted pyrolysis has gained attention as an efficient alternative capable of converting polyolefin-rich waste into valuable gaseous, liquid, and solid products.

Experimental: Silicon carbide (SiC) (Green Silicon Carbide, 2–4 mm, Sinabuddy Mineral, Zhengzhou, China), activated carbon (AC) (coconut shell-based, 6 × 12 mesh, Legend Inc., Sparks, NV, USA), and virgin polypropylene (PP) and polyethylene (PE) granules were sourced from Romcolor, Copăceni, Romania. In addition, polypropylene waste from automotive dismantling and two types of mixed polyolefin waste-comprising polypropylene and polyethylene, were collected from car components supplied by SC Pieseauto Dez SRL, Constanța, Romania.

Results and discussions: The highest performance was achieved for the PP and PP+PE samples, which exhibited elevated hydrogen concentrations and corresponding Gross Heating Values (GHV) of 54,320.32 kJ/kg and 55,087.35 kJ/kg, respectively. In all other experiments, the produced gas mixtures still demonstrated GHVs exceeding those of conventional fuels such as kerosene and diesel. From an environmental perspective, the specific CO_2 emissions of the pyrolysis-derived gases were generally lower or at least comparable to those of commercial fossil fuels.

* Corresponding author: grigore.psenovschi@icechim.ro

Conclusions: Microwave-assisted pyrolysis demonstrates strong potential for generating cleaner gaseous products with notably high Gross Heating Values (GHVs). The application of microwave energy promotes greater selectivity toward lighter hydrocarbons—compounds of high relevance in fuel upgrading—thereby providing a promising pathway for the production of more refined and energy-efficient fuels.

Acknowledgements: PN 23.06 Core Program-ChemNewDeal within the National Plan for Research, Development and Innovation 2022–2027, developed with the support of the Ministry of Research, Innovation, and Digitalization, project no. PN 23.06.01.01, AQUAMAT; and the Competitiveness Operational Program 2014–2020, Action 1.1.4: Attracting high-level personnel from abroad to enhance the RD capacity, project: P_37_471, "Ultrasonic/Microwave Nonconventional Techniques as new tools for nonchemical and chemical processes", financed by contract: 47/05.09.2016.

References:

[1] Barbeş, L., et al. Advancements in Automotive Waste Management. in CONAT 2024 International Congress of Automotive and Transport Engineering. 2025. Cham: Springer Nature Switzerland.

[2] Rovinaru, F.I., M.D. Rovinaru, and A.V. Rus, The Economic and Ecological Impacts of Dismantling End-of-Life Vehicles in Romania. Sustainability, **2019**. 11(22), 2071-1050, https://doi.org/10.3390/su11226446

.

SD-OP03 CO_2 CAPTURE AND CLIMATE POLICY DYNAMICS

Eliza-Gabriela Brettfeld[1,2*], Tănase Dobre[2*]

[1] INCDCP-ICECHIM Bucharest, 202 Spl. Independentei, 6th District, Romania

[2] UNST Politehnica Bucharest, Faculty of Chemical Engineering and Biotechnology

Abstract: *The study analyzes Europe's 2022–2025 energy transition, highlighting temporary fossil-fuel restarts and major CO_2-capture innovations that collectively advanced the EU's path toward climate-neutral industrial transformation.*

Key words: Carbon capture, utilization and storage CCUS; Energy geopolitics; Net-zero transition

Introduction: Carbon dioxide (CO_2) remains the main anthropogenic greenhouse gas, exceeding 420 ppm in 2025. The war in Ukraine and the resulting energy crises temporarily slowed the EU's decarbonization, as several Member States reactivated fossil-fuel power plants. Nevertheless, the European Commission maintained its 2030 target of capturing 50 Mt CO_2 annually through the 2024 Carbon Management Industrial Strategy and the REPowerEU plan.

Experimental and/or Modelling: The study integrates recent datasets from Eurostat, Ember, and the Global Energy Monitor, together with European Commission and IPCC reports (2022–2025). Comparative assessment of emissions and coal-plant restarts was used to evaluate the trade-off between energy security and climate objectives. Literature data from Stanford, the University of Surrey, and 8 Rivers supported the technological analysis of CO_2-capture innovation.

Results and Discussions: etween 2022 and 2025, around 13.5 GW of coal capacity were reactivated in nine EU states, raising coal's share to 13 % of the energy mix in 2023 (up from 9 % in 2021). Although this added roughly 220 Mt CO_2 in 2023, it stabilized energy supply during the crisis. From 2024 onward, programs like REPowerEU and Fit for 55 redirected over €65 billion into renewables and CCUS, reversing emission trends. Advances such as lithium–CO_2 batteries, accelerated mineralization, and graphene-based sorbents illustrate rapid scientific progress toward circular carbon management.

Conclusions: The 2022–2025 period represents a temporary regression followed by an unprecedented acceleration in low-carbon technologies, transforming CO_2 management into a cornerstone of Europe's climate-neutral industry.

Aknowledgement: The research leading to these results has received funding from project PN.23.06.02.01 InteGral, Nucleu Program, funded by the Romanian Ministry of Education and Research, National Agency for Research.

References: **[1]** European Commission, EU Action to Address the Energy Crisis, Brussels, 2025.; **[2]** Global Energy Monitor (GEM), Boom and Bust Coal 2025 – Tracking the Global Coal Plant Pipeline, San Francisco (CA), 2025.; **[3]** D'Ecclesiis E.A.R., Levi E., Patriarca F., The Impact of Ukraine's War Outbreak on Green Preferences in Europe, Ambio, 54 (6), 1095–1102 (2025).

* Corresponding author: mihaila.eliza.gabriela@gmail.com

* Corresponding author: tghdobre@gmail.com

SD-OP04 SYNERGISTIC MIXTURES OF GREEN CORROSION INHIBITORS FOR STEEL ANTICORROSION COATINGS

Ioana Maior* [1], Elena-Alexandra Duță[2], Emilia-Ioana Toma[2], Anca Cojocaru[1], Ioana-Alina Ciobotaru[1]

[1] Department of Inorganic Chemistry, Physical-Chemistry & Electrochemistry, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology POLITEHNICA Bucharest, 1–7 Gheorghe Polizu Str., 011061-Bucharest, Romania

[2] Faculty of Entrepreneurship, Engineering and Business Management, National University of Science and Technology POLITEHNICA Bucharest, 313 Independence Str., 060042-Bucharest, Romania

Abstract: *Corrosion, a spontaneously natural irreversible degradation process, affects metallic materials when interact with their environment (humidity, oxygen, salts, or acids). The objective of this work is to determine whether simple walnut extract (Junglas Regia JR) and in mixture with garlic extract (Allium Sativum AS), in various concentrations and ratios, could be efficiently used as inhibitor for carbon steel in corrosive acid medium. Thus, the experimental results suggest that the natural extracts investigated act on both partial reactions. Based on corrosion rate evaluation by gravimetric method, the efficiency of the simple inhibitors JR and AS, and respectively of the mixture of JR and AS, in different concentrations, in acidic H_2SO_4 medium, on carbon steel was evaluated: the simple JR extract reaches a maximum effectiveness of 51.56% (concentration 500 µL), at 24 hours immersion time, respectively 77.95% for AS, while the mixture of JR : AS, at a ratio of 1000 : 1000 µL, increases to an efficiency value of 85.51%.*

Key words: corrosion, green plant extract, synergistic mixtures, steel, acid environment

Introduction: Corrosion process is a major challenge for all industries, and for environmental protection, because it affects the safety of equipment and generates considerable economic losses [1, 2]. This experimental study involves weight loss measurements and specific electrochemical techniques, to evaluate the corrosion rates and inhibition efficiency values, for single and synergistic mixtures of hydroalcoholic plant extracts (JR, AS). The investigations focused on comparing the effectiveness of both eco-friendly corrosion inhibitors, single and in mixtures, in protecting carbon steel immersed in acid solution. The aim was to quantify the reduction in the corrosion rate of steel under the action of these extracts and to compare the performance of the inhibitors, revealing the level of protection provided by tested natural inhibitors and identifying the optimal usage conditions.

Experimental: To evaluate the corrosion rate and the inhibition efficiency of the natural plant extracts investigated, gravimetric method of metal samples weight loss was used, after a certain exposure time in the corrosion environment. The experiment was carried out on carbon steel metal samples, in 1N H_2SO_4 solutions, with / without natural inhibitor, simple / in mixtures of different ratios (Table 1). Electrochemical studies were performed with a Radiometer Analytical Voltalab 40

* Corresponding author: maior_i@yahoo.com

potentiostat, and a double-walled glass three-electrode electrochemical cell.

Results and discussions: According to the calculated data and based on the resulting curves, the corrosion rates decrease sharply in the first 14 days for the control solution as for the lower concentrations of inhibitor mixtures, while at high concentrations and ratios they tend to slightly increase. Then, in the following weeks, the corrosion rates tend to decrease slightly for all tested inhibitor concentrations, reaching a constant value. The inhibition efficacy values for both types of simple extracts increase with increasing inhibitor concentration but decrease significantly with increasing immersion time. For any of the concentrations of the inhibitor mixture, a significant increase in protective efficiency is observed compared to the use of simple extracts, which shows the synergistic nature of the inhibitor mixture.

Table 1. Efficiency of natural inhibitors on steel corrosion in acidic environment: comparison between simple extracts of JR, AS and the mixture of JR + AS, depending on the exposure time

H_2SO_4 + JR, µL	Inhibitor efficiency, EI, %	H_2SO_4 + AS, µL	Inhibitor efficiency, EI, %	H_2SO_4 + JR + AS, µL	Inhibitor efficiency, EI, %	Time, days
500	51.56	**500**	77.95	**500 (+400)**	78.81	1
	6.69		4.56		11.18	28
1000	48.71	**1000**	84.93	**1000 (+1000)**	85.51	1
	3.61		2.41		25.32	28

Conclusions: Many inhibitors in the mixture do not behave according to the rule of additivity but show an increase (synergism) or decrease (antagonism) in the individual effects, which do not depend on the amount of inhibitor added. Natural JR extract acts as an effective inhibitor, due to its polyphenolic compounds that adsorb on the metal surface and form a protective film. The addition of AS extract, rich in organosulphur compounds, enhances the inhibitory effect, by providing additional active compounds, with the possibility of a synergistic effect. Hence, a protective film is formed on the electrode surface, by the adsorption of organic compound molecules from the composition of the natural extract. The adsorption of inhibitors to the metal surface can affect the corrosion rate in two ways: by decreasing the active surface of the tested metal, or by modifying the activation energy of the anodic / cathodic reactions.

References:

[1] Haldhar, R., Prasad, D. & Saxena, A., Armoracia rusticana as sustainable and ecofriendly corrosion inhibitor for mild steel in 0.5M sulphuric acid: Experimental and theoretical investigations, *Journal of Environmental Chemical Engineering*, 6, (2018), 5230–5238

[2] Dehghani, A., Bahlakeh, G., Ramezanzadehb, B. & Ramezanzadeh, M., Potential of Borage flower aqueous extract as an environmentally sustainable corrosion inhibitor for acid corrosion of mild steel: Electrochemical and theoretical studies, *Journal of Molecular Liquids*, 277, (2019), 895–911

SD-OP05 EVALUATION OF QUINCE WINE PRODUCTION PROCESS AND FRUIT WINE CHARACTERIZATION

Ana - Maria Brezoiu[1,*], Florin - Cristian Tănase, Adrian - Marian Mitrică

[1] National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnology, 1-7 Gh. Polizu street, Bucharest, Romania.

Abstract: *Quince wines were prepared and analyzed and the proposed process is feasible.*
Key words: quince wine production, statistical analysis, chemical profile, economic evaluation

Introduction: Globally, a new interest in fruit-based alcoholic beverages was shown due to fruit wine novel sensory experiences and benefic compounds [1]. This study highlights the quince (*Cydonia oblonga)* wine production altogether with analytical characterization, microbiological control, and sensory evaluation to establish a well-defined platform for possible industrial manufacturing. Also, an economic evaluation was performed to support process feasibility.

Experimental: Quince fruits: a commercial cultivar from Turkey and a bio-certified Romanian cultivar, fresh or in frozen form were used. The quince juice and sucrose were mixed and subsequent inoculated with *Saccharomyces cerevisiae var. bayanus* and fermented in two stages. Comprehensive analyses of the final wines included alcohol content, titratable acidity, residual sugar, total soluble solids and polyphenols, sulfite content, antioxidant activity as well as wine chemical profile through HPLC-PDA.

Results and discussions: The quince wines presented alcohol levels between 12.1-15 °alc., residual sugars between 3.2-83.8 g/L and sulphites levels of 4.1-20.5 mg/L. Microbiological assays confirmed less than 1 colony of yeast and mold proliferation in the final products. Principal component analysis highlights the fruit wine with the best properties regarding analytical analysis or chemical profile. Sensory evaluation described the flavor, aroma, color, as well as overall acceptability. An opinion survey was conducted and more than 85% of the respondents would buy the tested product (quince wine). The economic evaluation showed a good feasibility for quince wine production plant with a profit of 1.5 million RON/year at 110 000 bottles sold annually.

Conclusions: Quince wine production confirms its physicochemical quality, microbiological safety, consumers' taste adaptability and process feasibility.

References:

[1] He L., Yan Y., Wu M., Ke L. Advances in the Quality Improvement of Fruit Wines: A Review. *Horticulturae* 2024, 10, 93.

* Corresponding author: ana_maria.brezoiu@upb.ro

SD-OP06 EVALUATION OF BIOCHEMICAL METHANE POTENTIAL OF DIFFERENT LIGNOCELLULOSIC SUBSTRATES

Elisabeta-Irina Geana*, Andreea Adelina Constantin, Corina Teodora Ciucure, Claudia Sandru, Florian Marin, Irina Petreanu, Roxana Elena Ionete

National Research and Development Institute for Cryogenics and Isotopic Technologies, Uzinei Str. No. 4, 240050 Ramnicu Valcea, Romania

Introduction: Lignocellulosic by-products derived from agricultural residues and woody biomass constitute a promising renewable feedstock for biogas generation due to their high carbohydrate content and abundance [1]. However, their recalcitrant structure, dominated by lignin–cellulose complexes, limits biodegradability during anaerobic digestion, thus requiring pretreatment in order to improve the methane yield [2]. This study evaluated the Biochemical Methane Potential (BMP) of various lignocellulosic substrates subjected to different pretreatment strategies to enhance anaerobic biodegradability and methane yield.

Experimental: Representative agricultural residues (wheat straw -WS and corn straw – CS) and woody biomass (beech sawdust – BS and spruce sawdust – SS) were characterized for their cellulose, hemicellulose, and lignin content, and their theoretical methane potential (BMP_{th}) was calculated using the Buswell equation. The substrates were then subjected to physical, chemical, and alkaline pretreatments to improve digestibility prior to batch anaerobic digestion The biochemical methane potential (BMP) of each sample was evaluated using an automatic methane potential system (AMPTS), using sludge from the sewage treatment plant as inoculum, at an inoculum-to-substrate ratio of 2, under mesophilic conditions (temperature 37 ◦C, retention time 30 days). Operating parameters such as total solids and volatile solids were gravimetrically measured. Specific methane yields (SMYs), as well as the theoretical methane potential (BMP_{th}), were used to calculate the biodegradability of the substrates. The gas composition analysis of the resulted biogas was performed by gas chromatography with thermal conductivity detection (GC-TCD).

Results and discussions: Results revealed that pretreatment significantly increased methane production by promoting the disruption of lignocellulosic structures and improving the accessibility of fermentable carbohydrates. The highest biodegradability was observed for WS (89 %) and CS (100 %) after the alkaline pretreatment, while, in the case of BS and SS the biodegradability was lower, with values of 75 % and 57 %, respectively (Figure 1). High-cellulose and low-lignin substrates, such as WS and CS exhibited the greatest methane yields, with values between 298.45-369.67 NmL CH_4/g VS in the case of WS and between 217.06-431.16 NmL CH_4/g VS. Lignin-rich materials such as BS and SS still remained

* Corresponding author: irina.geana@icsi.ro

recalcitrant, the obtained methane yields ranging between 164.24-310.99 NmL CH_4/g VS in the case of BS and between 123.31-234.66 NmL/g VS, indicating that for woody biomass stronger alkaline pretreatment is required.

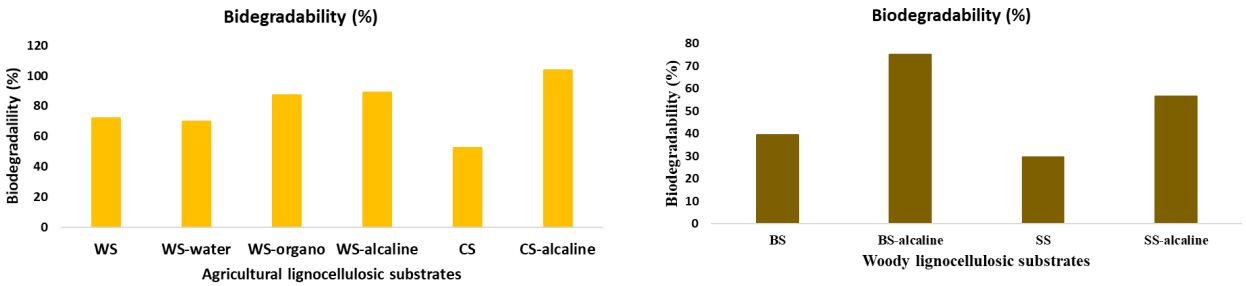


Figure 1. Biodegradability (%) of raw and pretreated agricultural and woody lignocellulosic substrates

Conclusions:

The comparison between theoretical and experimental BMP values highlighted the efficiency of each pretreatment method in enhancing substrate conversion. Agricultural residues exhibit higher BMP compared with woody biomass. Overall, the study demonstrates that appropriate pretreatment selection is crucial for maximizing biogas recovery from lignocellulosic feedstocks and improving the sustainability of anaerobic digestion processes.

Key words: lignocellulosic biomass, agricultural residues, woody biomass, anaerobic digestion, biofuels

Acknowledgments: This research was funded by the Romanian Ministry of Research, Innovation and Digitization through NUCLEU Program, Contract no. 20N/05.01.2023, Project PN 23 15 04 01: "The cascade valorisation of agro-industrial waste of plant biomass type in bioproducts with added value in the circular bioeconomy system".

References:

[1] F. J. Ngabala and J. K. Emmanuel, "Potential substrates for biogas production through anaerobic digestion-an alternative energy source," *Heliyon*, vol. 10, no. 23, p. e40632, Dec. 2024, doi: 10.1016/j.heliyon.2024.e40632.

[2] R. Agregán *et al.*, "Anaerobic Digestion of Lignocellulose Components: Challenges and Novel Approaches," *Energies*, vol. 15, no. 22, p. 8413, Jan. 2022, doi: 10.3390/en15228413.

SD-OP07 SIMULATION INSIGHTS INTO ETHANOL-TO-BUTADIENE PROCESS

Irina Maria Ariton, Romuald Győrgy, Ionuț Banu

Department of Chemical and Biochemical Engineering, Faculty of Chemical Engineering and Biotechnologies, POLITEHNICA Bucharest, 1-7 Gh. Polizu, Bucharest, Sector 1 011061

Abstract: *This work investigates the economic feasibility of producing butadiene from ethanol in a single step within a reaction-separation-recycle system based on economic potential. The key elements in determining the operating condition region that leads to process feasibility are the costs associated with the reaction stage, including catalyst regeneration, and those related to the recovery and reuse of unconverted reactants as well as the inert component. The approach in this study, validated through process simulation using the commercial simulator Aspen Plus v14, showed that the designed chemical process is robust if the amount of inert used is limited.*
Key words: Butadiene synthesis, Lebedev process, internal diffusion, economic potential

Introduction: For the transformation of ethanol into butadiene (ETB), two processes were developed in the early decades of the 20th century: the single-step process, developed by Lebedev, and the two-step process, developed by Ostromislensky, both abandoned after 1960. In the last decades, interest in these processes has been revived, especially through research focused on discovering more active, selective, and stable catalysts [1].

Modelling: In an initial approach, and considering that evaluating the effectiveness factor at the catalyst pellet level is a key activity when scaling up the process from laboratory to industrial level [1], this parameter was assessed for different catalyst pellet sizes, followed by a conceptual design of the process aimed at determining the mass of catalyst required to achieve a high butadiene yield. The conceptual design of the ETB process was carried out using Aspen Plus v14 simulator.

Results and discussions: Economic feasibility was assessed through four progressive levels, incorporating raw material costs, reaction costs, internal recirculation, and investment estimates via Aspen Plus simulations. The process becomes viable at an inert fraction of 0.2 and catalyst weight above 24 tons, for a butadiene annual production of 60 000 t/yr.

Conclusions: The findings emphasize the need for detailed process design, considering both transport phenomena at the granule level and optimization of reactor and recirculation configurations. Applying these principles enhances process efficiency and economic performance in butadiene production via the Lebedev process.

References:

[1]. Bozga G, Brosteanu AV, Banu I, Dimian AC (2024) One-stage ethanol to butadiene process: analysis and design of a multi-tubular fixed bed reactor. Chemical Engineering Research and Design 203:608-618. doi:https://doi.org/10.1016/j.cherd.2024.01.070

SD-OP08 BIOREFINERY APPROACH TO PRODUCE BIOENERGY, FOOD AND HIGH VALUE PRODUCTS FROM MOROCCAN SEAWEED *CYSTOSEIRA BACCATA*

Sabir Ibtissam[1,2,3*], Soumia Zaim[3], Rchid Halima[1,4], Christinne Gardarin[2], Philippe Michaud[2], Guillaume Pierre[2], Pierre Fontanille[2], Forano Claude[5], Ursu Alina-Violeta[2], El Moznine Reddad[3], Vial Christophe[2], Nmila Rachid[1,6]

[1]Biotechnology and Valorization of Vegetal Resources, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco

[2]Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, F-63000 Clermont-Ferrand, France

[3]Laboratory Physics of Condensed Matter, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco

[4]Polydisciplinary Faculty of Sidi Bennour, Chouaib Doukkali University, El Jadida, Morocco

[5]Université Clermont Auvergne, CNRS, Institut de Chimie de Clermont-Ferrand, F-63000 Clermont-Ferrand, France

[6]High School of Education and Training, Chouaib Doukkali University, El Jadida, Morocco

Abstract: *Seaweed are a sustainable renewable biomass for biorefinery applications. They can be cultivated without requiring agricultural land or chemical fertilizers, and contribute to atmospheric CO_2 mitigation, while yielding a wide spectrum of high value bioproducts. This study highlights the biorefinery potential of the brown seaweed Cystoseira baccata collected on the Moroccan Atlantic coast. The species exhibit high moisture content (83.4%) and a substantial mineral fraction (23.7% dry weight), with a balanced C/N ratio (15.0) favorable for bioconversion. Biochemical analysis revealed significant polysaccharide yields, with 10.5% alginate-rich and 3.2% fucoidan-rich fractions. These polysaccharides showed notable antioxidant activities in DPPH, FRAP, and hydroxyl radical scavenging assays, confirming their bioactive potential. Furthermore, the biomethane production potential (BMP) of the seaweed powder reached 1065 Nm^3 CH_4/t of organic weight while the extraction residues maintained a substantial yield of 697 Nm^3 CH_4/t organic weight, indicating the feasibility of energy recovery from by-products. Overall, C. baccata is a promising feedstock for integrated biorefinery systems, enabling the simultaneous production of high-value bio compounds and renewable bioenergy.*

Keywords: biorefinery, bioenergy, polysaccharides, alginates, fucoidans, *Cystoseira baccata*.

Introduction: *Cystoseira* (*Phaeophyceae*) is a genus of brown seaweeds widely distributed along temperate and subtropical coasts, including the Moroccan Atlantic shoreline. Owing to their distinctive *Cystoseira* sp. produce diverse bioactive metabolites such as fucoidans and alginates, that display multiple biological activities, making *Cystoseira* a promising source for various applications [1]. **Experimental:** Biological material and chemicals: Cystoseira baccata was collected from Sidi Bouzid coast (El Jadida, Morocco), then washed, dried in the dark at 45 °C, ground to a powder, and

* Corresponding author: ibtissam.sabir@doctorant.uca.fr

sieved. Moisture and ash content were determined gravimetrically: moisture by drying at 110°C for 48 h to constat weight, and ash by calcination at 550°C for 3 h. Elemental analysis (C, H, N, S) were performed with a Thermo Scientific FLASH SMART CHNS/O analyzer equipped with a Thermo Scientific MAS 200R sample holder and using BBOT *(2,5-bis(5-tert-butyl-2-benzoxazolyl)thiophene* as a calibration standard. The sequential extraction and characterization of fucoidans and alginates fraction were carried out according to the protocols described by Hentati et al. [2]. *A*ntioxidant activity was evaluated by the methods reported by Sabir et al. [3]. The Biochemical Methane Potential (BMP): was measured using the protocol proposed by Cresson et al. [4].

Results and discussions: The ash content (23.7% dry weight) indicates a significant mineral fraction, reflecting the seaweed ability to accumulate salts and trace elements from seawater. Elemental analysis showed a predominance of carbon (32.4%) and oxygen (35.5%), followed by hydrogen (4.5%), nitrogen (2.2%), and sulfur (1.4%), yielding a C/N ratio of 15.0, suggesting a favorable balance of organic carbon and nitrogen for microbial conversion processes. The gross calorific value (12.58 $MJ.kg^{-1}$ dry weight) denotes a moderate energy potential relative to terrestrial biomass. Regarding polysaccharide extraction, *C. baccata* contained 3.2% fucoidan-rich (Fuc.) and 10.5% alginate-rich (Alg.) fractions, confirming its suitability as feedstock for high-value bioactive polysaccharides in an integrated biorefinery. The antioxidant potential of Fuc. and Alg. extracted from *C. baccata* was assessed through DPPH, FRAP, and hydroxyl radical scavenging assays HRSA (Fig. 1). All samples exhibited concentration-dependent antioxidant effects. In the DPPH assay, both polysaccharides showed strong radical-scavenging activity, with Fuc. achieving 100% inhibition at 2 mg/mL. Alg. also inhibited DPPH, though with a lower intensity. FRAP results displayed a monotonic increase in absorbance with concentration, confirming the electron-donating capacity of both fractions. In HRSA assays, Alg. achieved 100% inhibition at 1 $mg.mL^{-1}$, consistent with efficient radical neutralization and metal chelation effects. Overall, Fuc. and Alg. possess significant antioxidant properties, likely associated to their sulfate (Fuc.) and carboxylate (Alg.) functionalities, which enhance reducing power and radical-scavenging behavior.

The algal powder exhibited a higher BMP (1065 Nm^3 CH_4/ton of organic matter) than the extraction residues (697 Nm^3 CH_4/ton of organic matter), indicating a loss of biodegradable material during extraction. This decrease aligns with the drop in organic matter (OM) content from 62.5% to 43.0% and the increase in mineral matter (MM) from 28.0% to 46.5%. The lower OM/MM ratio (48.0% *vs.* 69.1%) further confirms depletion of fermentable compounds. Despite this reduction, the extraction residues maintain a moderate methane potential, suggesting scope for valorization through anaerobic digestion.

Conclusions: *Cystoseira baccata* exhibits strong potential for marine biorefinery applications. Its composition enables both the extraction of antioxidant polysaccharides (fucoidans and alginates) and bioenergy production through anaerobic digestion. Even after extraction, the residues retain a valuable energy potential, confirming the suitability of this species for integrated valorization that couples bioproduct and biofuel production.

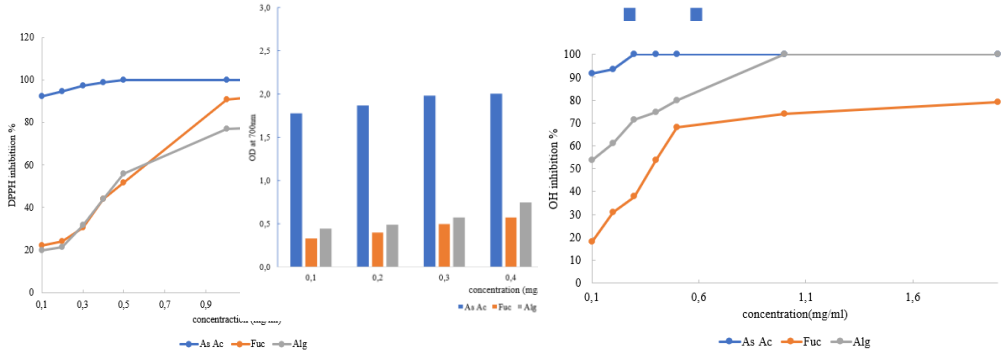


Fig. 1: Antioxidant activities of fucoidans-rich (Fuc.) and alginates-rich fraction (Alg.) compared to ascorbic acid (As Ac) by DPPH, FRAP, and HRSA

References:

[1]. De Sousa et al., *Cystoseira algae* (*Fucaceae*): update on their chemical entities and biological activities Carolina. *Tetrahedron: Asymmetry*, 28, (2017), 1486-1505.

[2]. Hentati F. et al., Structural characterization and antioxidant activity of water-soluble polysaccharides from the Tunisian brown seaweed *Cystoseira compressa*, *Carbohydr. Polym*., 198, (2018), 589-600.

[3]. Sabir I. et al., Crudes polysaccharides from *Cystoseira* species: Extraction, Characterization and *in vitro* Antioxidant Activity. *Natural Product Sciences*. 31(2): 102-110 (2025).

[4]. Cresson R., Pommier S., Béline F., Bouchez T., Bougrier C., Buffière P., Cacho, J., Camacho P., Mazéas L., Pauss A. (2014). Etude Interlaboratoires pour L'harmonisation des Protocoles de Mesure du Potentiel Bio Methanogène des Matrices Solides Hétérogène. Rapport Final, ADEME Paris, Fr. 1–121.

BOOK OF ABSTRACTS

SICHEM – 2025

D – Green applied chemistry and agro-resources valorization (GACARV)

2. Poster presentations

SD-P01 EVALUATION OF LIPOSOMAL CAROTENOID FORMULATIONS WITH POTENTIAL USE IN FUNCTIONAL FOOD SYSTEMS

Violina Popovici[1,*], Eugenia Covaliov, Tatiana Capcanari, Oxana Radu, Alexandrina Cojocari

[1]Technical University of Moldova, Faculty of Food Technology, Food and Nutrition Department, 9/9 Studentilor str., MD-2045, Chisinau, Republic of Moldova

Abstract: *Carotenoids are natural lipophilic pigments with strong antioxidant potential, widely recognized for their role in reducing oxidative stress and promoting health. Their integration into functional food systems is, however, limited by low stability and poor bioavailability due to their sensitivity to environmental and processing conditions. Liposomal encapsulation offers a promising strategy to overcome these limitations by improving carotenoid protection, stability, and controlled release [1]. This study focused on the characterization of liposomal formulations loaded with carotenoids extracted from Hippophae rhamnoides powder and on evaluating their potential use in functional food applications. Spectrophotometric analysis of the sea buckthorn extract revealed the presence of significant amounts of carotenoids 9.9 ± 0.03 mg/100 g. Liposomes were prepared using a modified Mozafari method [2,3], followed by extrusion through 100 nm membranes to enhance homogeneity. The resulting emulsions exhibited a high encapsulation efficiency (92.80±1.25%) and a retention rate of 90.2±2.08 %, confirming the effectiveness of the encapsulation process. Particle size analysis showed that, before extrusion, the liposomal formulations exhibited a mean diameter of 195.72 ± 6.61 nm, which decreased to 154.72 ± 3.53 nm after extrusion. This reduction in size was accompanied by a significant improvement in particle uniformity, confirming that the extrusion step plays a crucial role in producing stable and homogeneous vesicles suitable for incorporation into food systems. To assess practical applicability, the liposomal emulsions were incorporated into biscuit formulations, and their in vitro antioxidant activity was evaluated under simulated gastrointestinal conditions. The biscuits containing encapsulated carotenoids showed significantly higher antioxidant activity than those with non-encapsulated extracts, particularly under gastric conditions (94.8±1.68% vs. lower values for free extracts). Liposomal encapsulation effectively protected carotenoids from oxidative and digestive degradation, maintaining substantial antioxidant potential throughout the digestion process.*

The results demonstrated that liposomal encapsulation is a highly effective strategy for improving the stability and bioavailability of sea buckthorn carotenoids. The formulated liposomal systems exhibited favorable physicochemical properties, strong antioxidant activity, and excellent retention of bioactive compounds during storage and digestion. These findings highlight the potential of liposomal carotenoid formulations as functional ingredients in the development of innovative food products with enhanced nutritional and health-promoting properties.

Key words: encapsulation, bioactive compounds, antioxidant activity, quality.

Acknowledgments: The research was supported by the State Project for Young Researchers 25.80012.5107.10TC "Stabilization of Plant-derived Bioactive Compounds by Liposomal Encapsulation", running within Technical University of Moldova.

References: [1] Liu, P.; Chen, G.; Zhang, J. A Review of Liposomes as a Drug Delivery System: Current Status of Approved Products, Regulatory Environments, and Future Perspectives. Molecules 2022, 27, 1372.; [2] Rasti, B.; Jinap, S.; Mozafari, M.R.; Yazid, A.M. Comparative Study of the Oxidative and Physical Stability of Liposomal and Nanoliposomal Polyunsaturated Fatty Acids Prepared with Conventional and Mozafari Methods. Food Chem. 2012, 135, 2761–2770.; [3] Popovici, V.; Boldianu, A.-B.; Pintea, A.; Caraus, V.; Ghendov-Mosanu, A.; Subotin, I.; Druta, R.; Sturza, R. In Vitro Antioxidant Activity of Liposomal Formulations of Sea Buckthorn and Grape Pomace. Foods 2024, 13, 2478. https://doi.org/10.3390/foods13162478

* Corresponding author: Email address: violina.popovici@toap.utm.md

SD-P02 MICROWAVE-ASSISTED EXTRACTION OF POLYPHENOLS FROM *CRATAEGUS MONOGYNA* L.

Anca M. Roșca, Ioan Călinescu, Ioana Popa, Adina I. Gavrilă*

[1]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology *Politehnica* Bucharest, 011061 Bucharest, Romania

Abstract: *Hawthorns (Crataegus monogyna L.) contain numerous bioactive compounds, with its extracts demonstrating health benefits. This study focused on optimizing a more sustainable extraction method, specifically microwave-assisted extraction (MAE), to obtain polyphenols from hawthorn leaves and flowers. HPLC/UV analysis identified key compounds, while principal component analysis (PCA) assessed correlations between extraction conditions, total phenolic content (TPC), and key compounds.*

Key words: hawthorn; bioactive compounds; microwave-assisted extraction

Introduction: In recent years, consumers have tended towards natural and eco-friendly products related to pharmaceuticals, food, cosmetology, and agronomy. Hawthorn contains polyphenols, terpenoids, lignans, organic acids, nitrogenous compounds, and vitamins [1-2]. The recovery of these can be achieved through their extraction using both conventional and unconventional methods.

Experimental: Polyphenols were extracted from powdered plant material using a MW applicator, under various conditions in regards to solvents, solvent-to-plant ratio, temperature and time. The TPC was determined using the Folin–Ciocalteu assay [3]. A two-level factorial analysis was performed on three variables.

Results and discussions: MAE was compared with conventional extraction, yielding higher TPC when using MAE. The optimal operating conditions for MAE are typically determined through statistical optimization studies. The screening of 3 independent variables: solvent-to-plant ratio (S/P = 10–30 mL/g), temperature (t = 50–70 °C), and ethanol concentration (EtOH = 25–75%) was conducted using 2^3 factorial design. Optimal MAE conditions (S/P_{opt} = 20.4 mL/g, T_{opt} = 65 °C, and $EtOH_{opt}$ = 60%) yielded a TPC of 116.23 ± 2.85 mg GAE/g DM and an AA of 237.6±6.33 mg TE/g DM using hawthorn leaves and flowers.

Conclusions: The resulting hawthorn extracts, enriched with polyphenols, could be used in dietary supplements to prevent neurodegenerative diseases.

Acknowledgment: This work was supported by GNAC ARUT 2023, project: FitoNeuroPro", code 179, no. 4/06.10.2023.

References:

[1] Martinelli, F. et al. Botanical, phytochemical, anti-microbial and pharmaceutical characteristics of hawthorn (*Crataegus monogyna* Jacq.), Rosaceae. *Molecules* 26, (2021), 7266.

[2] Guo,W.; et al. Chemical composition, biological activities, and quality standards of hawthorn leaves used in traditional Chinese medicine. *Front. Pharmacol*. 14, (2023), 1275244.

[3] Gavrila, A.I.; et al. Green extraction techniques of phytochemicals from *Hedera helix* L. and in vitro characterization of the extracts. *Plants* 12, (2023), 3908.

* Corresponding author: adina.gavrila@upb.com

SD-P03 ASSESSMENT OF TRANS FATTY ACID INTAKE DURING TRADITIONAL ROMANIAN MEALS

Beatrice C. Poteraș[1,2], Fulvia Manolache[2], Adina I. Gavrilă[1], Cristina Todașcă[1,*]

[1]Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology Politehnica Bucharest, 1-7 Gh. Polizu Street, 011061 Bucharest, Romania

[2]National Research & Development Institute for Food Bioresources—IBA, 5 Ancuța Băneasa Street, 020323 Bucharest, Romania

Abstract: *This study assesses compliance with the regulatory limit of trans fatty acids in the context of traditional Romanian festive meals. Knowing the negative effect of the trans fatty acid on the consumers health this research aims to examinate the risk of exposing consumers to large amounts of trans fatty acid, higher of the regulated limits, when traditional meals are consumed.*
Key words: trans fatty acid; food products; traditional meals; FT-IR

Introduction: Trans-fatty acids (TFAs) can may occur either naturally from raw materials used in food formulation or be generated during technological processing [1]. Regulation (EU) 2019/649 was introduced by the European Union as a public measure, setting a maximum limit of 2 g of industrial trans fatty acids per 100 g of fat in food products [2].

Experimental: Fat extraction from food products was carried out using Soxhlet method. FT-IR-ATR spectrometry was applied to both fat samples and calibration standards (glyceryl trioleate and glyceryl trielaidate mixtures) to determine the trans fatty acid content [3].

Results and discussions: In Romania, Christmas and Easter meals include a wide range of meat-based and pastry dishes that may contribute substantially to dietary trans fatty acid intake. Food products such as cozonac, telemea cheese, panettone, Easter eggs, cabbage rolls were selected to illustrate the trans fatty acid content of foods typically consumed during traditional meals, such as Christmas and Easter. The quantification of trans fatty acids indicated variations associated with both product type and festive period. Particularly, the panettone sample exhibited the highest trans fatty acid concentration among the analyzed products, likely due to the specific fat composition of the formulation.

Conclusions: Consequently, within the context of a traditional festive meal, the intake of trans fatty acids remains within the legally established limits.

References:

[1] Nagpal T. et al. Trans fatty acids in food: A review on dietary intake, health impact, regulations and alternatives. *Journal of Food Science*, 86, 12, (2021), 5159-5174.

[2] Commission Regulation (EU) 2019/649 of 24 April 2019 (2019), https://eur-lex.europa.eu/legal-content/RO/TXT/?uri=CELEX:32019R0649&qid=1715422965357

[3] Manolache F.A. et al. Influence of Edible Oil Variety on Trans Fatty Acids Formation During the Frying Process, Revue Roumaine de Chimie, 67, (2022), 93–99.

* Corresponding author: cristina.todasca@upb.com

SD-P04 ASSESSMENT OF CHRONIC EXPOSURE AND RISK ASSOCIATED WITH THE CONSUMPTION OF CEREALS AND CEREAL PRODUCTS BY DETECTING THE HEAVY METAL CONTENT

Corina A. Stroe[1,2], Gabriel Mustățea[2], Elena L. Ungureanu[2], Andreea L. Mocanu[1,2], Adina I. Gavrilă[1], Mihaela Tociu[1,*]

[1]Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology POLITEHNICA Bucharest, 011061 Bucharest, Romania

[2]National Research and Development Institute for Food Bioresources – IBA Bucharest, 020323 Bucharest, Romania

Abstract: *Cereals and cereal-based products are a major component of the human diet and represent an important source of energy. However, due to their frequent consumption, contamination with heavy metals may pose significant health risks, particularly under chronic exposure conditions. This study aimed to assess the concentrations of eight heavy metals in wheat flour samples collected from 41 counties across Romania.*
Key words: wheat flour; heavy metals; ICP-MS; health risks; Romania

Introduction: Cereals are an important food source for people worldwide and provide valuable nutrients such as carbohydrates, proteins, fibers, minerals, vitamins and phytochemicals. Regular consumption of whole grains is associated with a lower risk of chronic diseases such as cancer, type 2 diabetes and cardiovascular disorders. In contrast, refined cereals offer fewer health benefits due to their lower nutrient content [1].

Experimental: Wheat flour from 41 Romanian counties was homogenized, dried, and milled to a uniform particle size. Samples were digested using HNO_3, 65% and H_2O_2, 30% under controlled temperature and pressure. The resulting solutions were analyzed by ICP-MS, a sensitive and accurate technique to detect trace metal, to determine the concentrations of Pb, Cd, Cr, Cu, Zn, Mn, Co, and Ni [2].

Results and discussions: ICP-MS analysis revealed notable regional variability in heavy metal content across Romania. The highest concentrations of Pb, Cd, Cu, and Zn were found in Arad, Alba, Constanta, Galati, and Giurgiu, mainly linked to industrial and agricultural activities. Lower contamination levels were observed in Neamt, Olt, and Salaj, reflecting cleaner environmental conditions.

Conclusions: The results reveal regional contamination differences, necessitating stronger monitoring and food safety for cereal-based products.

References:

[1] Garutti M., Nevola G., Mazzeo R., Cucciniello L., Totaro F., Bertuzzi C.A., Caccialanza R., Pedrazzoli P., Puglisi F., The Impact of Cereal Grain Composition on the Health and Disease Outcomes, *Front. Nutr.*, 9, (2022), 888 - 974.

[2] Ungureanu E. L., Mustățea G., *Toxicity of Heavy Metals, Environmental Impact and Remediation of Heavy Metals*, IntechOpen, 2022.

* Corresponding author: mihaela.tociu@upb.ro

SD-P05 FERMENTATION-DRIVEN REDUCTION OF ANTINUTRITIONAL FACTORS AND IMPROVEMENT OF MINERAL BIOAVAILABILITY IN LEGUME–CEREAL SYSTEMS

Eugenia Covaliov*, Violina Popovici, Tatiana Capcanari, Oxana Radu

Food and Nutrition Department, Technical University of Moldova

Abstract: *The present study explores the potential of controlled microbial fermentation to enhance the nutritional and functional properties of mixed substrates derived from legumes (lentils, peas), cereals (rye, oats), and pseudocereals (quinoa, amaranth). These plant matrices are rich in proteins, fibers, phenolics, and minerals, but their nutritional value is limited by the presence of antinutritional compounds such as phytates and tannins, which bind divalent cations and reduce the bioavailability of essential micronutrients, particularly iron and zinc.*

To overcome these limitations, lactic fermentation was applied using selected probiotic strains — Lactobacillus plantarum *and* Lactobacillus casei *— known for their strong phytase, β-glucosidase, and polyphenol-modifying activities. Fermentation conditions (pH 5.5–6.0, 35 °C, 24–48 h) were optimized to stimulate enzymatic degradation of phytates and hydrolysis of tannin–protein complexes, while preserving the integrity of proteins and phenolic antioxidants.*

Chemical analyses revealed a reduction of 45–70 % in phytic acid content and a notable decrease in total tannins (30–55 %), accompanied by a 30–60 % increase in soluble iron and zinc fractions. The molar ratio of phytic acid to iron dropped below the critical threshold (10:1), indicating improved mineral bioaccessibility. In parallel, fermentation promoted the release of free phenolic acids (such as ferulic and gallic acids) and enhanced the antioxidant capacity measured by DPPH and FRAP assays.

The microbial metabolism of L. plantarum *and* L. casei *also contributed to mild acidification and exopolysaccharide formation, which improved the viscosity and sensory attributes of the fermented blends. The resulting matrices displayed a pleasant slightly acidic flavor and smooth texture, suitable for the formulation of plant-based yogurt-like beverages and fermented snacks with high biological value. These findings demonstrate that lactic fermentation is an effective bioprocess for transforming legume–cereal substrates into functional foods with enhanced mineral bioavailability and antioxidant properties. The approach provides a sustainable technological solution aligned with the principles of the circular bioeconomy, enabling the conversion of diverse plant resources into nutritious, microbiologically stable, and consumer-acceptable products.*

Key words: *Lactobacillus plantarum*, *Lactobacillus casei*, fermentation, phytates, tannins, iron bioavailability, legumes, cereals, pseudocereals

* Corresponding author:

SD-P06 SMART FERTILIZERS FROM CHROMIUM TANNED LEATHER WASTE

Ana-Maria Nicoleta Codreanu (Manea) [1], Daniela Simina Stefan [2*], Rachid Aziam[3], Lidia Kim[4]

[1] PhD student, Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology Politehnica of Bucharest, Gheorghe Polizu Street, No. 1-7, Bucharest, Romania

[2] Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology Politehnica of Bucharest, Gheorghe Polizu Street, No. 1-7, Bucharest, Romania

[3] Laboratory of Applied Chemistry and Environment, Department of Chemistry, Faculty of Science, Ibnou Zohr University, BP 8106 Agadir, Morocco

[4] National Research and Development Institute for Industrial Ecology, Department for Evaluation, Monitoring Environmental Pollution, Drumul Podu Dambovitei Street, No 57-73, ZIP Code 060652, Bucharest, Romania

Abstract: *Smart fertilizers represent one of the most recent and innovative categories of fertilizers, offering a sustainable alternative to conventional formulations. The incorporation of collagenic waste from the leather industry into smart fertilizer compositions has emerged as a topic of significant interest within the field. Gelatin, derived from leather waste, exhibits several advantageous properties including biodegradability, low toxicity, and hydrophilicity, which make it suitable for applications in smart fertilizers, either as an encapsulating matrix or as a direct nutrient source (containing 11–14% nitrogen). The development process of smart fertilizers based gelatin integrates biotechnology and biodegradable materials to enable the controlled release of nutrients to plants. This approach not only enhances nutrient use efficiency but also minimizes the environmental impact associated with traditional fertilization practices.*

The present study introduces a new method for obtaining smart fertilizers derived from chromium-tanned leather waste by applying the circular economy principles. The experimental work was based on four main stages: chromium extraction, hydrolysis, nutrient enrichment and crosslinking. The preliminary chromium extraction step, carried out using oxalic acid, EDTA and distilled water, was essential due to the high chromium content of the tanned leather sample (~3.5%). At the hydrolysis step using a leachate ash : water ratio of 1:2 at 100 °C, a collagen hydrolysate containing 12.5% nitrogen and 9.3% potassium was obtained. The resulting hydrolysate was then enriched with an alternative phosphorus source and subsequently subjected to the crosslinking process. To enhance the controlled-release efficiency, the fertilizer was further crosslinked with an additional source of gelatin (stirred at 45 °C for 12 hours). Fertilizer granulation was achieved by dripping the solution into a cold oil bath. After 24 hours, the granules were separated from the oil phase by vacuum filtration and washed with ethanol and water
Keywords: *Smart fertilizer, circular economy, leather waste, collagenic waste*

[*] Corresponding author: daniela.stefan@upb.ro
anamariacodreanu99@yahoo.com, rachid.aziam@edu.uiz.ac.ma; lidia.kim@incdecoind.ro

SD-P07 UNMODIFIED WASTE EGGSHELLS: SUITABLE BIOMATERIALS FOR THE REMOVAL OF HEAVY METALS

Elena Petronela Bran[1], Oana-Irina Patriciu[2], Luminița Grosu[2], Irina-Claudia Alexa[2*], Brîndușa Bălănucă[3], Adrian-Ionut, Nicoară[4] and Adriana-Luminița Fînaru [2*]

[1]Doctoral School, "Vasile Alecsandri" University of Bacău, 157, Calea Mărășești, 600115 Bacău, Romania;

[2]Department of Chemical and Food Engineering, Faculty of Engineering, "Vasile Alecsandri" University of Bacău, 157, Calea Mărășești, 600115 Bacău, Romania;

[3]Department of Organic Chemistry "C. Nenitescu", Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7, Gheorghe Polizu Street, 011061 Bucharest, Romania;

[4]Department of Science and Engineering of Oxide Materials and Nanomaterials, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7, Gheorghe Polizu Street, 011061 Bucharest, Romania;

Abstract: *Eggshells represent a suitable biosorbent for the adsorption of heavy metals due to their composition and bioavailability. This study was carried out in order to evaluate the absorption capacity of untreated chicken and quail eggshells for the removal of Pb and Zn ions from aqueous solutions using four types of agitation systems: classical and orbital agitation and ultrasonic and microwave-assisted activation. The results of this study contribute to providing solutions in sustainable waste management, through the recycling of this type of biomaterial.*
Key words: heavy metal; biosorption; agitation-activation system; eggshells;

Introduction: A well-known application of eggshells is their use as biomaterials with adsorption properties for the removal of heavy metals from contaminated waters [1]. The agitation/activation system can influence the bioadsorption process of heavy metal ions. The appropriate choice of the agitation mode may maintain high adsorption capacities, while reducing time and energy consumption.

Materials and Methods: Chicken and quail eggshells and their 1 : 1 (*w/w*) mixture were used to investigate the removal capacity of Pb and Zn ions from aqueous solutions. Four types of agitation/activation systems were tested for the adsorbent solution samples: classical and orbital agitation, ultrasonic, and microwave activation. The monitoring of aqueous solutions and morpho-structural characteristics of eggshell powder samples before and after the adsorption process was performed using various electrochemical and spectro-analytical techniques [2].

Results and Discussions: All types of unmodified eggshells proved a good capacity for the removal of Pb and Zn ions from aqueous solutions. In the case of chicken eggshells, their removal efficiency for the lead ions was 65% and for the zinc ions over 80%, regardless of the type of agitation and temperature. Concerning the Zn removal

* Corresponding author:

efficiency of quail eggshells, noteworthy results were recorded when microwaves were applied (>90%) and at 40 °C for orbital shaking and ultrasound (>80%) [2].

Conclusions: The results of this study reveal the advantages of agitation/activation systems applied to different types of unmodified eggshells that can be used as an adsorbent for heavy metals, being appropriate for a sustainable management of waste.

Acknowledgements: The authors are grateful for the support accorded by "Vasile Alecsandri" University of Bacău through the projects CNFIS-FDI-2025-F-0483 and SSD-0153-2025 and also for the access to the research infrastructure of the National Center for Micro and Nanomaterials through the National Program titled "Installations and Strategic Objectives of National Interest".

References:

[1] Ahmed, T.A.; Wu, L.; Younes, M.; Hincke, M. Biotechnological Applications of Eggshell: Recent Advances. *Front. Bioeng. Biotechnol.* **2021**, 9, 675364. https://doi.org/10.3389/fbioe.2021.675364

[2] Bran, E.P.; Patriciu, O.-I.; Grosu, L.; Alexa, I.-C.; Bălănucă, B.; Nicoară, A.-I.; Fînaru, A.-L. The Influence of Different Parameters for the Removal of Pb and Zn Ions on Unmodified Waste Eggshells. *Materials* **2025**, 18, 2794. https://doi.org/10.3390/ma18122794

SD-P08 PURSUING INNOVATIVE AND SUSTAINABLE APPROACHES FOR THE VALORIZATION OF POMACE

Luminiţa Grosu[1], Daniela Nicuţă[2], Oana-Irina Patriciu[1], Irina-Claudia Alexa[1*], Adriana-Luminiţa Fînaru[1]

[1]Department of Chemical and Food Engineering, Faculty of Engineering, "Vasile Alecsandri" University of Bacău, 157, Calea Mărășești, 600115 Bacău, Romania;

[2]Department of Biology, Faculty of Sciences, "Vasile Alecsandri" University of Bacău, 157, Calea Mărășești, 600115 Bacău, Romania;

Abstract: *The waste from wine industry represents an important environmental issue at national level as well as worldwide. Our research team has expressed its interest in investigations concerning the reuse of grape pomace, with the aim of finding innovative and sustainable ways to valorize them in different areas. The results of our research may contribute to providing solutions in sustainable waste management, through the valorization of this type of biomaterial.*
Key words: pomace; powder; extracts; valorization; functional food; plant growth

Introduction: Grape pomace, due to its composition rich in polyphenols, exhibits numerous important biological activities such as antioxidant, antimicrobial, antifungal and anti-inflammatory. From these considerations, grape pomace can represent a valuable bioresource with applications in the food industry, cosmetics, medicine, etc. Our research has focused both on the food sector, by incorporating the grape pomace powder to obtain functional food products [1], and at the same time towards the field of biotechnology, by investigating the potential application of the grape pomace extracts on *in vitro* plant growth and development [2].
Materials and Methods: Honey-based product and dehydrated apple and banana fruit rolls enriched with different proportion of *Fetească Neagră* grape pomace powder were prepared. Some physico-chemical parameters of the samples were investigated and hedonic-scale method was used for the sensorial analysis. On the other hand, different concentrations of grape pomace extracts were added in the *in vitro* culture medium of *Origanum vulgare*. The morphogenetic response of the shoots obtained on the tested experimental variants was recorded and compared to the control group.
Results and Discussions: The results of the study indicate that the grape pomace powder can be used as functional ingredient for the development of honey-based products and dehydrated apple and banana fruit rolls, contributing to a sustainable process innovation. Following the sensory analysis, the products obtained a high degree of acceptability. Regarding the influence of grape pomace hydroalcoholic extracts on the regeneration processes of *Origanum vulgare* explants inoculated *in vitro*, it was highlighted that the stimulatory effect on the morphogenetic response

* Corresponding author:

depends both on the extraction method used and on the proportion in which the nutrient medium was supplemented with grape pomace extracts.

Conclusions: The results of this research reveal that grape pomace still represents a by-product of interest for researchers, offering permanently innovative and sustainable approaches for its valorization.

Acknowledgements: The authors are grateful for the support accorded by "Vasile Alecsandri" University of Bacău through the project CNFIS-FDI-2025-F-0483.

References:

[1] Suceveanu, E.-M.; Grosu, L., Alexa, I.-C.; Fînaru, A.: Valorisation potential of *Fetească neagră* grape pomace for obtaining honeybased fortified innovative product, *Scientific Study & Research - Chemistry & Chemical Engineering, Biotechnology, Food Industry* **2020**, 21 (2), 243-252.

[2] Bran, P.E.; Nicuţă, D.; Grosu, L.; Patriciu, O.-I.; Alexa, I.C.: Investigation regarding the potential application of grape pomace extracts on *in vitro* plant growth and development, *Ovidius University Annals of Chemistry* **2022**, 33 (2), 135-142. https://doi.org/10.2478/auoc-2022-0020

SD-P09 AGROWASTE UTILIZATION FOR THE DEVELOPMENT OF WATER-SOLUBLE FOOD PACKAGING

Andra-Gabriela Zorcă, Alessia-Ioana Enescu, Ion Sorin Jinga, Cristina Busuioc, Iuliana Mihaela Deleanu*

Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology POLITEHNICA Bucharest, 1-7 Gh. Polizu, 011061 Bucharest, Romania

Abstract: *The development of sustainable food packaging material is necessary not only to minimize the environmental pollution, but also to enhance food quality for the consumers.*
There are many strategies, approaches and methods towards food waste and lost reduction and one of them is the development of bio-based products, fabricated from renewable raw resources and/or by utilization of food by-products, and food waste [1, 2]. Usage of food by-products and food waste not only reduce the environmental, societal, and economic burden, but also could bring the benefits of their contained bioactive compounds [3]. Thus, by innovative processing, new high-end products with specific functionalities, besides inherent biocompatibility and biodegradability, can be obtained. It is the case of sustainable food packaging materials that could improve not only the way that food is packed, but also the way it is consumed [4].
In this research, various composites based on polyvinyl alcohol and Mung bean peel have been developed. Preliminary tests indicate acceptable water vapor permeability for the composites, while being fully soluble in water.
Key words: polyvinyl alcohol, beans peel, biodegradability, waste valorization

References:

[1] Ansari, S. A., Kumar, T., Sawarkar, R., Gobade, M., Khan, D., & Singh, L., Valorization of food waste: A comprehensive review of individual technologies for producing bio-based products. J. Environ. Manag., vol. 364, 121439, (2024), https://doi.org/10.1016/j.jenvman.2024.121439.
[2] Dima, A. D., Pârvulescu, O. C., Mateescu, C., & Lungulescu, E. M., Influence of gamma-ray irradiation on the biomethane production of sunflower seed cake, U.P.B. Sci. Bull., Series B, 83 (1), (2021), 59-72.
[3] Egri, D., Cristina Pârvulescu, O., Alexandra Ion, V., Moloșag, A., Dobrin, A., Moț, A., Orbeci, C., Dobre, T., Bormac, I., Løes, A.-K., Cabell, J., & Salifoglou, A. (2024). Preparation and characterization of compost tea derived from rockweed residues. U.P.B. Sci. Bull., Series B, 86 (3), (2024), 123-134.
[4] Hassoun, A., Boukid, F., Ozogul, F., Aït-Kaddour, A., Soriano, J. M., Lorenzo, J. M., Perestrelo, R., Galanakis, C. M., Bono, G., Bouyahya, A., Bhat, Z., Smaoui, S., Jambrak, A. R., & Câmara, J. S., Creating new opportunities for sustainable food packaging through dimensions of industry 4.0: New insights into the food waste perspective, Trends Food Sci. Technol., Vol. 142, 104238, (2023), https://doi.org/10.1016/j.tifs.2023.104238.

* Corresponding author: iuliana.deleanu@upb.ro

SD-P10 COMPOSITION AND ANTIOXIDANT ACTIVITY OF SEA BUCKTHORN FRUIT EXTRACTS

Ionela Otilia Baciu[1*], Oana Cristina Pârvulescu[1], Violeta Alexandra Ion[2], Mihaela Tociu[1], Nicoleta Chira[1]

[1]National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnology, 1-7 Gheorghe Polizu St., 011061 Bucharest, Romania

[2]Research Center for Studies of Food Quality and Agricultural Products, University of Agronomic Sciences and Veterinary Medicine Bucharest, 59 Marasti Blvd., 011464 Bucharest, Romania

Abstract: *This study aimed at establishing the effects of extraction process factors on the composition and antioxidant activity of sea buckthorn (Hippophae rhamnoides L.) fruit extracts. Microwave-assisted extraction (MAE) tests were conducted under different operating conditions, using mixtures of ethanol and water as extraction solvents. Solvent/vegetal material ratio (15–30 mL/g DM) and ethanol/water ratio (1–4 mL/mL) were selected as process factors. Total phenolic content, total flavonoid content, and antioxidant activity were experimentally determined and predicted at different levels of MAE factors. Process optimization was performed based on the desirability function approach.*

Key words: antioxidant activity; microwave-assisted extraction (MAE); optimization; phenolic compounds; sea buckthorn (*Hippophae rhamnoides* L.).

Introduction: Sea buckthorn (SB) berries contain different natural antioxidants, *e.g.*, phenolic compounds (phenolic acids, flavonoids, tocopherols), carotenoids (*β*-carotene, *γ*-carotene, lycopene, zeaxanthin, lutein), ascorbic acid (vitamin C), which exhibit antioxidant, antimicrobial, anti-inflammatory, and anticancer effects [1–5]. The valorization of (SB) berries and residues resulting from their processing (seeds, skin, and pulp residues) represents a major opportunity for the development of food, nutraceutical, cosmetic, and pharmaceutical products with added value [6].

Experimental and modeling: MAE of bioactive compounds from dried and ground SB berries was performed in a Multiwave PRO Microwave Reaction System (Anton Paar, Graz, Austria). MAE tests were conducted at 60 ºC, using mixtures of ethanol and water as extraction solvents. Liquid/solid ratio (R_{LS} = 15–30 mL/g DM) and ethanol/water ratio (R_{EW} = 1–4 mL/mL) were selected as process factors. The extracts were analyzed to determine total phenolic content (*TPC*), total flavonoid content (*TFC*), and antioxidant activity, evaluated as percentage of inhibition of DPPH (2,2-diphenyl-1-picrylhydrazyl) free radical (*PI*). Second-order polynomial models were used to quantify the effects of the process factors on *TPC*, *TFC*, and *PI*. The optimal levels of the process factors were obtained based on the desirability function approach [7].

* Corresponding author: baciu.otilia@yahoo.com

Results and conclusions: The values of the experimental response variables were in the following ranges: *TPC* = 4.597–10.44 mg CAE/mg DM, *TFC* = 5.585–11.59 mg QE/g DM, and *PI* = 23.51–50.54%, where CAE represents the caffeic acid equivalents, QE the quercetin equivalents, and DM the dry matter. The profiles of the predicted response variables highlighted the following:
- an increase in *TPC*, *TFC*, and *PI* with an increase in R_{LS} for R_{LS} = 18.75–30 mL/g DM and almost constant values for R_{LS} = 15–18.75 mL/g DM;
- a decrease in all response variables with an increase in R_{EW} for R_{EW} = 2.5–4 mL/mL and almost constant values for R_{EW} = 1–2.5 mL/mL.
The optimal levels of the process factors were $R_{LS,opt}$ = 30 mL/g and $R_{EW,opt}$ = 1.5 mL/mL. The predicted optimal values of process response variables ($TPC_{pr,opt}$ = 10.48 mg CAE/mg DM, $TFC_{pr,opt}$ = 11.63 mg QE/g DM, and $PI_{pr,opt}$ = 50.76%) were in a good agreement with the experimental values (TPC_{opt} = 10.44 ± 0.21 mg CAE/mg DM, $TFC_{,opt}$ = 11.59 ± 0.34 mg QE/g DM, and $PI_{pr,opt}$ = 50.54 ± 1.67%), and the optimal value of desirability function was 0.9.
SB extracts prepared under optimal operating conditions could be used as ingredients in food, nutraceutical, cosmetic, or pharmaceutical products.

References:

[1] Gâtlan, A. M., Gutt, G., Sea buckthorn in plant based diets. An analytical approach of sea buckthorn fruits composition: Nutritional value, applications, and health benefits, *International Journal of Environmental Research and Public Health*, 18, 17, (2021), 8986.
[2] Ion, V. A., Pârvulescu, O. C., Velcea, D., Popa, O., Ahmadi, M., Physico-chemical parameters and antioxidant activity of Romanian sea buckthorn berries, *Revista de Chimie*, 70, 12, (2019), 4187–4193.
[3] Jaśniewska, A., Diowksz, A., Wide spectrum of active compounds in sea buckthorn (*Hippophae rhamnoides*) for disease prevention and food production, *Antioxidants*, 10, 8, (2021), 1279.
[4] Michalak, M., Plant-derived antioxidants: Significance in skin health and the ageing process, *International Journal of Molecular Sciences*, 23, 2, (2022), 585.
[5] Wang, Z., Zhao, F., Wei, P., Chai, X., Hou, G., Meng, Q., Phytochemistry, health benefits, and food applications of sea buckthorn (*Hippophae rhamnoides* L.): A comprehensive review, *Frontiers in Nutrition*, 9, (2022), 1036295.
[6] Bal, L. M., Meda, V., Naik, S. N., Satya, S., Sea buckthorn berries: A potential source of valuable nutrients for nutraceuticals and cosmoceuticals, *Food Research International*, 44, 7, (2011), 1718–1727.
[7] Drăghici-Popa A. M., Boscornea A. C., Brezoiu A. M., Tomas Ș. T., Pârvulescu, O. C., Stan, R., Effects of extraction process factors on the composition and antioxidant activity of blackthorn (*Prunus spinosa* L.) fruit extracts, *Antioxidants*, 12, 10, (2023), 1897.

SD-P11 GREEN CHEMISTRY APPLICATIONS IN THE SEPARATION OF NEUROPROTECTIVE ALKALOIDS FROM *NARCISSUS* SPECIES

Cristina Anca Secara [1], Mihaela Dragoi Cudalbeanu[2], Diana-Mihaela Popescu[1], Vladimir Suhaianu[1], Claudia-Valentina Popa[1,3*]

[1]„Cantacuzino" National Military Medical Institute for Research and Development, 103 Splaiul Independenței, 050096, Bucharest, Romania

[2]University of Agronomic Sciences and Veterinary Medicine of Bucharest, 59 Marasti Boulevard, 011464 Bucharest, Romania

[3]University of Bucharest, 90 Sos Panduri, 030018 Bucharest, Romania

Abstract: *Isolation of galantamine from the vegetable raw material, through technologies with low environmental impact was carried out.*

Key words*:* green chemistry, galantamine, *Narcissus poeticus* extract, neuroprotection

Introduction: Galantamine is a tertiary alkaloid used in the treatment of Alzheimer's disease. The aim of the project consists of isolation of galantamine from the plant extracts, through technologies with low environmental impact.

Experimental and/or Modelling: A extract obtained by microwave technique from *N. poeticus* was quantitatively analyzed by an HPLC-PDA system, with: the Symmetry C18 column (250 x 4.6 mm, 5 μm), set at 30 °C; the injection volume 20 μL; elution flow rate 1 mL/min.; the mobile phases (A) 0.1 % formic acid (FA) in water and (B) 0.1 % FA in acetonitrile in the elution gradient, wavelength 288 nm. The separation of galantamine was performed by CPC technique. The compound's neuroprotection was evaluated by the MTT cell viability assay.

Results and discussions: Separation of galantamine using centrifugal partition chromatography revealed a purified fraction with a high content of galantamine (1.25 mg/kg) with a recovery of 68.36%. Exposure to the organophosphorus compound in a rat hippocampal neuron cell line pretreated with the studied compound in concentration of 12 μg/mL, revealed main values of cell viability of 91.37% ± 14 (galantamine from natural extract) and 89.16% ± 9 (galantamine obtained through chemical synthesis), values that do not differ statistically significant ($p = 0.3$; $n_1 = n_2 = n_3$, Student´s T test).

Conclusions: The obtaining of galantamine from extracts, respects the principles of green chemistry. The neuroprotective effect of natural galantamine is comparable to the synthetized one.

References:

[1] Birks J.S. Cholinesterase inhibitors for Alzheimer's disease. *Cochrane Database Syst Rev*., 1 (2006), CD005593.

* Corresponding author: popa.claudia@cantacuzino.ro

SD-P12 EQUIVALENT ELECTRICAL CIRCUITS IN ELECTROCHEMICAL SYSTEMS: STEEL IN 3.5% NACL SOLUTION IN THE PRESENCE OF APIUM GRAVEOLENS EXTRACT

Anca Cojocaru*, Claudia Irimia, Marian Stoica, Ioana Alina Ciobotaru, Ioana Maior

[1]National University of Science and Technology Politehnica Bucharest, Faculty of Chemical Engineering and Biotechnologies, 1-7 Gh. Polizu St., sect. 1, 011061, Bucharest, Romania

Abstract: *Electrochemical impedance spectroscopy (EIS) is an important tool for the evaluation of corrosion of metallic materials. In this work the evaluation of corrosion inhibition of steel in 3.5% NaCl solution in the presence of Apium Graveolens (AG) extract by EIS measurements was presented. An electric equivalent circuit was proposed.*

Key words: Steel corrosion, electrochemical impedance spectroscopy, equivalent circuit, Apium Graveolens (AG) extract

Introduction: Steel corrosion is a major and costly problem faced by many industries worldwide. According to Mansfeld [1], corrosion is a problem that can be monitored by means of electronic devices that apply an electrical signal (V or I) to measure and control the transfer of electrical charge to evaluate the reaction kinetics and the mechanism of the corrosion process that takes place at the metal/solution interface. Electrochemical impedance spectroscopy (EIS) is a commonly employed method for analyzing the characteristics of electrochemical systems. The typical method for evaluating EIS measurements is to use equivalent electrical circuits [2,3]. When used appropriately, they can offer a rough mechanistic understanding of the electrochemical system under consideration. The model is chosen to provide the best possible match between the model impedance and the measured impedance.

Experimental: The system studied consisted of a carbon steel working electrode (surface area of 1 cm^2), a platinum gauze used as a counter electrode and Ag,AgCl/KClsat (SSCE) reference electrode immersed directly in the working solution using a 50 mL electrochemical cell. The electrolyte was 3.5% NaCl solution obtained from p.a. chemical reagent and distilled water to which different concentrations of *Apium Graveolens (AG)* extract (purchased from the market) were added. The experiments were performed at room temperature (22°C) using Voltalab 40 Radiometer Analytical potentiostat/galvanostat with VoltaMaster 4.0 software for data acquisition. Electrochemical impedance spectroscopy (EIS) studies were performed at open circuit potential in the frequency range 100 kHz–100 mHz with a sinusoidal potential perturbation of 10 mV amplitude.

Results and discussions: The model of equivalent circuit proposed to fit the EIS experimental data for steel corrosion in 3.5% NaCl solution in the presence of

* Corresponding author: anca.cojocaru@upb.ro

Apium Graveolens (AG) extract was a Randles type circuit. The circuit consisted of a solution resistance (R_s), a double layer capacitor C_{dl} (or a constant phase element) connected in parallel with a charge transfer resistance (R_{ct}). The extract was added to the electrolyte solution in the concentration range 500 - 4000 ppm. The inhibition efficiency, calculated from charge transfer resistance obtained from Nyquist plots, had values ranging from 79.97% to 92.67%. The highest value of inhibition efficiency, 92.67%, was obtained for the highest studied value of *AG* extract.

Conclusions: The studied *Apium Graveolens* extract proved to be a promising source for the development of a natural inhibitor to combat corrosion, and further research could give more information about the mechanism of the action of this extract in protecting metallic materials against corrosion.

References:

[1] Mansfeld F. Don't Be afraid of electrochemical techniques — But use them with care. Corrosion Science. 1988;44(12):856-868. DOI: 10.5006/ 1.3584957

[2] Wang, F. S., Li, Y., Zhang, Y. X., & Chen, G. Y. (2020). A method to select the optimal equivalent electrical circuit applied to study corrosion system of composite coating on magnesium alloy. *Physics Letters A*, *384*(24), 126452.

[3] Van Haeverbeke, M., Stock, M., & De Baets, B. (2022). Equivalent electrical circuits and their use across electrochemical impedance spectroscopy application domains. *Ieee Access*, *10*, 51363-51379.

SD-P13 THEORETICAL FOUNDATIONS OF GOLD(III) RECOVERY FROM CHLORIDE MEDIA USING AQUEOUS POLYETHYLENE GLYCOL SYSTEMS

A. M. Lăcătuş*, L. Bulgariu

[1]Gheorghe Asachi Technical University of Iasi, Faculty of Chemical Engineering and Environmental Protection, 73 D. Mangeron Street, 700050, Iasi, Romania

Abstract: *This paper presents an evaluation of aqueous two-phase systems (ATPS) composed of polyethylene glycol (PEG) and ammonium sulfate for the selective extraction of Au(III) from chloride-containing solutions. The influence of variables such as PEG molecular weight, chloride ion concentration, and pH on extraction efficiency were systematically studied. Results indicate that gold primarily forms tetrachloroaurate complexes preferentially partitioning into the PEG-rich phase. Extractions exceeding 98% were achieved at acidic pH and chloride concentrations above 0.08 mol/L. Application on industrial waste samples demonstrates the potential of this environmentally friendly approach for effective gold recovery.*

Key words: Au(III), aqueous two-phase systems, polyethylene glycol, chloride ions, selective extraction)

Introduction: Selective recovery of Au(III) from aqueous media is essential due to the metal's economic and technological importance and environmental concerns regarding traditional extractants. Polymer-salt aqueous two-phase systems represent a promising alternative. This work systematizes experimentation on Au(III) extraction in PEG-$(NH_4)_2SO_4$ systems, focusing on parameters influencing phase partition behavior within chloride-rich matrices.

Experimental and/or Modelling: ATPS were prepared by mixing PEG (1500–6000 g/mol) and ammonium sulfate solutions. Au(III) chloride solutions with varying chloride content were synthesized. Extractions were conducted in batch mode at ambient conditions; phase separation was centrifugally facilitated. Gold concentrations were determined by atomic absorption spectrometry.

Extraction efficiency is quantified via the distribution coefficient K_d:

$$Kd = C_{PEG} / C_{salt}$$

Results and discussions : Extraction efficiency correlates positively with chloride concentration and PEG molecular weight, achieving values exceeding 98% at pH ≤ 3.0 and chloride levels above 0.08 mol/L. Interferences from other metal ions were minimal except for Fe(III), which exerted a minor influence at high chloride concentrations. Validation on real electronic waste leachates supported the method's applicability.

Selective extraction behavior is detailed in Figure 1, illustrating superior Au(III) recovery relative to competing ions under varying chloride ion concentrations.

* Corresponding author: andrei-marius.lacatus@student.tuiasi.ro

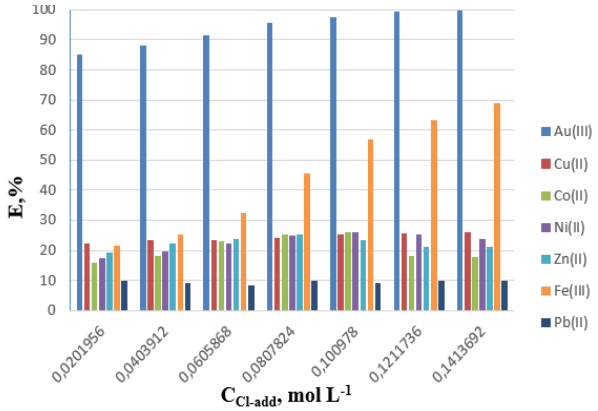


Fig. 1 The extraction percent of Au(III) and other metal ions as a function of chloride ions extractants concentration

Conclusions: PEG-$(NH_4)_2SO_4$ ATPS offer a versatile and sustainable platform for Au(III) separation from chloride media, with tunable parameters supporting selective and efficient extraction. These findings promote further development of green, scalable processes for precious metal recovery from secondary resources.

References:

[1] Bulgariu L., Bulgariu D., Extraction of gold(III) from chloride media in aqueous polyethylene glycol-based two-phase systems, Journal of Hazardous Materials, vol. 196, pp. 96–103, 2011
[2] J.O. Marsden, C.I. House, The Chemistry of Gold Extraction, second ed., Society for Mining, Metallurgy and Exploration Inc. (SME), Littleton, 2006.
[3] L. Bulgariu, D. Bulgariu, Possibility of using aqueous PEG(1500)– (NH4)2SO4 two-phase system for the extraction of heavy metal ions, Bull. I.P. Iasi, Chemistry and chemical engineering (in press).

SD-P14 TOPICAL OINTMENT CONTAINING A MIXTURE OF ECHINACEA PURPUREA AND ARMORACIA RUSTICANA EXTRACTS - A PHYTOTHERAPEUTIC APPROACH TO SKIN HEALTH

Ramona-Daniela Pavaloiu[1], Corina Bubueanu[1], Angela Casarica[1], Ciprian Fodor[2], Mariana Fodor[2], Roman Emilian[2], Diana-Ioana Cristea[3], Teodor-Mihai Florescu[3], Fawzia Sha'at[1*]

[1]National Institute for Chemical-Pharmaceutical Research&Development – ICCF, Bucharest, 112, Vitan Av., Bucharest, Romania

[2]SC PURE LIFE SRL, 13 Veronica Micle Street, Suceava, Romania

[3]Faculty of Pharmacy, University of Medicine and Pharmacy "Carol Davila", Traian Vuia Street, no. 6, sector 2, Bucharest, Romania

Key words: ointment, Echinacea purpurea, Armoracia rusticana, skin health

Introduction: *Echinacea purpurea* and *Armoracia rusticana*, widely recognized for their anti-inflammatory and skin-regenerative properties, have shown promise in dermatological applications.

Experimental: A phytotherapeutic ointment was formulated using *Echinacea purpurea* and *Armoracia rusticana* standardized hydroalcoholic extracts (30% ethanol) in a 1:1 ratio. The ointment base consisted of cocoa butter, shea butter, beeswax, lanolin, grape seed oil, calendula oil, vitamin E, triethanolamine and essential oils, aiming to enhance dermal delivery and therapeutic efficacy. Physicochemical characterization included pH analysis, texture profiling, and stability studies. *In vitro* release studies were performed using Franz diffusion cells and medium replacement (phosphate buffer, pH 5.8, temperature of 32 ^{0}C).

Results and discussions: Physicochemical characterization of the ointment revealed a dermo-compatible pH of 5.1 ± 0.02. Texture profile analysis confirmed good homogeneity and appropriate firmness for topical application. Stability testing over a three-month period indicated no signs of phase separation, discoloration, or changes in odor, demonstrating good formulation stability. *In vitro* release studies showed a sustained release of both plant extracts.

Conclusions: These promising results suggest the formulation is suitable for further biological evaluation. The combination of *Echinacea purpurea* and *Armoracia rusticana* may offer anti-inflammatory and antimicrobial benefits for topical applications. Further *in vivo* and microbiological testing is planned to confirm therapeutic potential.

Aknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0317, within PNCDI IV.

References: [1] Olivero-Verbel J, Quintero-Rincón P, Caballero-Gallardo K. (2024) Aromatic plants as cosmeceuticals: Benefits and applications for skin health. *Planta*, 260:132. https://doi.org/10.1007/s00425-024-04550-8; [2] Sitarek P, Kowalczyk T, Wieczfinska J, Merecz-Sadowska A, Górski K, Śliwiński T, Skała E. (2020). Plant extracts as a natural source of bioactive compounds and potential remedy for the treatment of certain skin diseases. *Curr Pharm Des.,* 26:2859–2875. https://doi.org/10.2174/1381612826666200714092704

* Corresponding author: fawzya.shaat@gmail.com

SD-P15 CHARACTERIZATION OF GRAPE POMACE FLOUR FOR OBTAINING VALUE-ADDED PRODUCTS

Georgiana Irina (Bercea) Vizitiu[1,2*], Alina Soceanu[2], Simona Dobrinas[2], Oana Cristina Parvulescu[3], Vasile Lavric[3]

[1] IOSUD Politehnica Bucharest, Doctoral School "Chemical Engineering and Biotechnologies"1-7 Gheorghe Polizu St., 011061, Bucharest, Romania,

[2] Department of Chemistry and Chemical Engineering, Ovidius University from Constanta, 124 Mamaia Blvd., Constanta, Romania,

[3] Chemical and Biochemical Engineering Department, National University of Science and Technology Politehnica Bucharest, 1-7 Gheorghe Polizu St., 011061, Bucharest, Romania.

Abstract: *Due to the large amount of waste generated every year from the wine industry and the high demand on the market for value-added products, the aim of this study was to investigate the characteristics of a category of waste, as grape pomace, to assess its potential for reuse in the food industry. The analysis was also based on research into the influence of pomace flour added to wheat flour in different concentrations of 2%, 4% and 7%. Following research, it has been demonstrated that raw pomace flour cannot be used alone in a pastry or bakery product from a technological point of view but must be attached to wheat flour to be effective.*
Key words: wine industry, waste, grape pomace, flour

Introduction: Grapes are one of the most widely grown fruit crops worldwide, but their processing in the wine industry leads to the generation of significant amounts of waste. Of these, pomace is the main by-product of the winemaking process. By transforming it into grape pomace flour, this residual material, with numerous nutrients can be exploited as a functional ingredient for the development of innovative food products [1],[2].

Experimental: Grape pomace samples were collected from different grape varieties originated from the Red Feteasca Neagra variety, from the Merlot Rose variety, and from the Chardonnay variety. The decision to select these grape varieties was supported by the distinct color differences among these samples. The samples collected were dried and subsequently analyzed in the laboratory from a physico-chemical perspective. In addition, a control sample of type 650 wheat flour was also analyzed. Parallel to this, further analyses were conducted on type 650 flour supplemented with different concentrations of 2%, 4%, and 7% of each pomace sample (Red Feteasca Neagra, Merlot Rose, and Chardonnay).

Results and discussions: As a result of the conducted study, it was found that, from a technological viewpoint, raw grape pomace flour cannot be used as such in the production of bakery or pastry products, due to the absence of certain essential compounds that contribute to the quality of these products. However, based on the

* Corresponding author: georgiana.bercea@365.univ-ovidius.ro

research carried out, it was demonstrated that a combination of type 650 wheat flour (control) with a 2% and 4% addition of grape pomace flour, regardless of the grape variety (Red Feteasca Neagra, Merlot Rose, or Chardonnay) is technologically feasible for use in the food industry.

Conclusions: Waste resulting from the winemaking process represents an important raw material resource, characterized by a significant potential for use in multiple industrial fields, including the food industry**.** The use of grape pomace is an alternative to reduce waste, improving sustainability [3].

References:

[1] G. Gurumeenakshi, P. Geetha and R. Rajeswari, *Utilization of grape pomace as a raw material for the development of value added products,* Int.J.Curr.Microbiol.App.Sci (2021) 10(03): 772-779;

[2] Jaqueline Menti Boff, Virgílio José Strasburg, Gabriel Tonin Ferrari, Helena de Oliveira Schmidt, Vitor Manfroi and Viviani Ruffo de Oliveira, *Chemical, technological, and sensory quality of pasta and bakery products made with the addition of grape pomace flour*, Foods 2022, 11, 3812;

[3] Artur Siller-Sánchez, Karla A. Luna-Sánchez,Israel Bautista-Hernández, Mónica L. Chávez- González., *Use of grape pomace from the wine industry for the extraction of valuable compounds with potential use in the food industry,* Current Food Science and Technology Reports (2024) 2:7–16.

SD-P16 COMPOSITION AND ANTIOXIDANT ACTIVITY OF EXTRACTS OF BASIL, CHICORY, AND COMMON SAGE

Grațiela Elena Popescu, Andreea Cristina Donise*, Oana Cristina Pârvulescu, Mihaela Emanuela Crăciun

[1]National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnology, 1-7 Gheorghe Polizu St., 011061 Bucharest, Romania

Abstract: *This study aimed at establishing the effect of extraction solvent on the composition and antioxidant activity of extracts of basil (O. basilicum), chicory (C. intybus), and common sage (S. officinalis) obtained by maceration under stirring.*
Key words: antioxidant activity; basil (*Ocimum basilicum*); chicory (*Cichorium intybus*); common sage (*Salvia officinalis*); extraction; flavonoids; phenolic compounds.

Introduction: Phenolic compounds, *e.g.*, flavonoids, phenolic acids, are plant secondary metabolites that have antioxidant and antimicrobial properties [1,2]. The extraction yields of secondary metabolites from plants and antioxidant activity of the extracts depend on different process factors, *e.g.*, extraction method, operating conditions, type of plant, extraction solvent, and equipment [1].

Experimental: Edible flower extracts were obtained through maceration under stirring (250 rpm), using a mixture of ethanol and methanol (containing 0%, 40%, 60%, and 100% ethanol) as extraction solvent. Total polyphenol content (*TPC*), total flavonoid content (*TFC*), and percentage of inhibition (*PI*) of basil, chicory, and common sage extracts were determined using specific techniques. The experimental data were processed using principal component analysis (PCA) and one-way ANOVA.

Results and conclusions: The extracts obtained from common sage had significantly higher mean values of *TPC* (48.53–64.21 mg GAE/mg DM), *TFC* (25.81–36.79 mg QE/mg DM), and *PI* (64.44–79.86%) than those prepared from basil (34.25–37.14 mg GAE/mg DM, 17.57–22.86 mg QE/mg DM, and 56.53–61.82%) and chicory (23.12–30.31 mg GAE/mg DM, 10.16–14.08 mg QE/mg DM, and 54.74–62.03%). The correlations between *TPC*, *TFC*, and *PI* were significant ($0.738 \leq r \leq 0.997$). These edible flower extracts could be used as ingredients in food, nutraceutical, or cosmetic products.

References:

[1] Do, Q. D., Angkawijaya, A. E., Tran-Nguyen, P. L., Huynh, L. H., Soetaredjo, F. E., Ismadji, S., Ju, Y. H., Effect of extraction solvent on total phenol content, total flavonoid content, and antioxidant activity of *Limnophila aromatica*, *Journal of Food and Drug Analysis*, 22, 3, (2014), 296–302.

[2] Zheng, J., Lu, B., Xu, B., An update on the health benefits promoted by edible flowers and involved mechanisms, *Food Chemistry*, 340, (2021), 127940.

* Corresponding author: andreeadonise@yahoo.com

SD-P17 PREPARATION, CHARACTERIZATION, AND TESTING OF MARINE RESIDUE-DERIVED FERTILIZERS/BIOSTIMULANTS

Andreea Nichitoi[1], Oana Cristina Pârvulescu[1,*], Violeta Alexandra Ion[2], Ailin Moloșag[2], Andrei Moț[2], Cristina Orbeci[1], Tănase Dobre[1], Anne-Kristin Løes[3], Joshua Cabell[3], Athanasios Salifoglou[4], Carlos Octavio Letelier-Gordo[5]

[1]Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology POLITEHNICA Bucharest, 1–7 Gheorghe Polizu St., 011061 Bucharest, Romania

[2]Research Center for Studies of Food Quality and Agricultural Products, University of Agronomic Sciences and Veterinary Medicine of Bucharest, 59 Marasti Blvd., 011464 Bucharest, Romania

[3]Norwegian Centre for Organic Agriculture, Gunnarsveg 6, NO-6630 Tingvoll, Norway

[4]School of Chemical Engineering, Aristotle University of Thessaloniki (AUTh), Corner of September 3rd and Egnatia St., 462, 54124 Thessaloniki, Greece

[5]National Institute of Aquatic Resources, DTU Aqua, Section for Aquaculture, Technical University of Denmark, 9850 Hirtshals, Denmark

Abstract: *This study aimed at upgrading poorly used marine residual materials by treating them using appropriate technologies to produce fertilizers and biostimulants. Compost derived from fish and rockweed (Ascophyllum nodosum) residues, compost tea obtained by compost fermentation, biochar impregnated with compost tea, and a biostimulant derived from macroalgae residues were prepared, characterized, and tested as ferilizers/biostimulants.*

Key words: biostimulant; compost; compost tea; fertilizer; fish residue; lettuce; rockweed (*Ascophyllum nodosum*) residue; strawberry.

Introduction: There is currently a strong interest in increasing the production of organic and high-quality food, especially vegetables and other horticultural products, supporting a healthy lifestyle, and protecting soil quality and biodiversity. Therefore, research is needed to design efficient and environmentally friendly fertilizers and biostimulants derived from sustainable residual biomass. Processing marine residues, which are currently underutilized, and producing fertilizers and biostimulants can have significant agronomic and environmental benefits. Fish bones and other fish residues, which are rich in P, Ca, and N, can be very valuable as fertilizers [1]. Macroalgae contain a wide range of nutrients required by plants, *e.g.*, K, Mg, S, microelements. Fertilizers based on fish and macroalgal residues can significantly enhance plant growth [1–3]. Also, materials derived from macroalgae can be used as biostimulants, to increase plant resistance to abiotic and biotic stress [4,5].

Experimental and results: Marine residual materials, *i.e.*, fish (cod, common ling, cusk, haddock, and saithe) heads and backbones from the clipfish industry and rockweed residues resulting from extraction processes, were analyzed. The relevant

* Corresponding author: oana.parvulescu@yahoo.com

physicochemical parameters, including the contents of macronutrients, micronutrients, fatty acids, and amino acids, were determined. The marine residues were then processed using appropriate methods (composting, fermentation, impregnation, and extraction), and several products were obtained:
(1) two types of compost, *i.e.*, CR, obtained by composting rockweed residues with LECA (lightweight expanded clay aggregate) in a reactor, and CW, prepared by windrow composting of fish and rockweed residues (at a volumetric ratio of 1:4.4) with woodchips;
(2) two types of compost tea (CTR and CTW) produced by fermenting both types of compost (CR and CW);
(3) wood-based biochar (BC) impregnated with CTR and CTW;
(4) a biostimulant derived from rockweed residues (BIO).
These products were analyzed and then tested for the growth and development of strawberry and lettuce. CW, BC impregnated with CTW, and BIO had similar or positive effects compared to commercial fertilizers and biostimulants.
Conclusions: The study provided new perspectives on residue reduction and full utilization of marine residual biomass toward production of efficient fertilizers and biostimulants. Recycling fish and rockweed residues using suitable techniques, *i.e.*, composting, fermentation, impregnation, and extraction, could have significant beneficial agronomic and environmental effects.

Acknowledgments:
This conference presentation is part of the project 244/2021 ERANET–BLUEBIO–MARIGREEN, which has received funding from the European Union's Horizon 2020 research and innovation program under agreement 817992 and Ministry of Research, Innovation and Digitization, CNCS/CCCDI–UEFISCDI, within PNCDI III.

References:

[1] Ahuja, I., Dauksas, E., Remme, J. F., Richardsen, R., Løes, A. K., Fish and fish waste-based fertilizers in organic farming–with status in Norway: A review, *Waste Management*, 115, (2020), 95–112.
[2] Moloșag, A., Pârvulescu, O. C., Ion, V. A., Asănică, A. C., Soane, R., Moț, A., Dobrin, A., Frîncu, M., Løes, A. K., Cabell, J., Salifoglou, A., Maroulis, M., Matsia, S., Bujor, O. C., Egri, D., Dobre, T., Bădulescu, L. A., Lagunosvchi-Luchian, V., Effects of marine residue-derived fertilizers on strawberry growth, nutrient content, fruit yield and quality, *Agronomy*, 13, 5, (2023), 1221.
[3] Riley, H., Effects of algal fibre and perlite on physical properties of various soils and on potato nutrition and quality on a gravelly loam soil in southern Norway, *Acta Agriculturae Scandinavica*, Section B-Plant Soil Science, 52, 2, (2002), 86–95.
[4] Du Jardin, P., Plant biostimulants: Definition, concept, main categories and regulation, *Scientia Horticulturae*, 196, (2015), 3–14.
[5] Verkleij, F. N., Seaweed extracts in agriculture and horticulture: A review, *Biological Agriculture & Horticulture*, 8, 4, (1992), 309–324.

SD-P18 CHROMATIC AND IMAGISTIC ANALYSIS OF BUCKWHEAT-ENRICHED BREAD

Vasilica-Alisa Aruș[1], Alin Teușdea[2], Ana-Maria Georgescu[1],
Nicoleta Vartolomei[3], Nicoleta Platon[1], Ileana-Denisa Nistor[1]

[1]"Vasile Alecsandri" University of Bacau, Faculty of Engineering, 157 Calea Marasesti, 600115 Bacau, Romania

[2]University of Oradea, Faculty of Environmental Protection, 26 Gen. Magheru St., 410048 Oradea, Romania

[3]Technological High School of Targu Ocna, Nicolae Arnabanas, 1-3, Targu Ocna, Bacau

Abstract: *Bread is one of the most important staple foods consumed by mankind throughout time. Since it is a staple food for many peoples and population categories, bread is often fortified to improve nutritional properties. Bread fortification is done by adding rye, rice, barley, oat, corn, buckwheat, millet flours, by adding potatoes or seeds, but also fruit powder, etc. The color of food is the first quality parameter evaluated by consumers and is essential in the acceptance of the product. In the present paper the chromatic and imagistic analysis was performed over bread without added buckwheat flour (BWF) and bread and with added buckwheat flour (BBWF) scanned image samples with six different extract concentrations (0 to 12.5 % BWF).*

Key words: buckwheat flour, bread formulation, colour image analysis, porosity of bread

Introduction: Food color is considered the most important factor for flavor perception; it sets consumers' expectations about what those food products will taste like, as well as the pleasure or distaste of experiencing those products [1].

Experimental: Whole buckwheat flour (BWF) was added (2.5; 5; 7.5; 10 and 12.5 % BWF) in white wheat flour in order to obtain different blends of flour. After baking, the bread was labelled and left for 3 h at room temperature for cooling, and then it was prepared for analysis (moisture, porosity and crumb elasticity) [1]. The investigated chromatic parameters were CIE L*a*b* and browning index (Bi). The imagistic analysis performed pixel classification with fifteen classes (C1 ÷ C15) based on chromatic criteria.

Results and conclusions:

The crumb and crust colour became darker with the level of wheat flour substitution. The internal structure of crumb became coarser, with irregular pores.

The results of the multivariate analysis prescribe a full discrimination between all the BBWF samples (i.e., each analysed sample consist in a singleton cluster), with exception of control and 2.5% samples that gather in a cluster.

References:

[1] Vasilica-Alisa Aruş, Ana-Maria Georgescu, Nicoleta Platon, Ana-Maria Roșu, Gabriela Muntianu, Alin Cristian Teușdea, Nicoleta Vartolomei, Ileana-Denisa Nistor, Preliminary studies concerning the influence of buckwheat flour on the quality of white wheat breadScientific Study & Research Chemistry & Chemical Engineering, Biotechnology, Food Industry, 2024, 25 (2), pp. 157 – 167.

SD-P19 THE RELATIONSHIP BETWEEN NUTRIENT CONCENTRATIONS AND PHYTOPLANKTON DEVELOPMENT(CHLOROPHYLL-A) IN THE SURFACE WATERS OF THE LOWER DANUBE RIVER

Daniela Florea[1], Dan Vasiliu[1], Vasile Lavric[2], Florentina Fediuc[1], Naliana Lupașcu[1], Albert Scrieciu[1]

[1]National Institute for Research and Development on Marine Geology and Geoecology – GeoEcoMar, 23–25 Dimitrie Onciul Str., 024053, Bucharest, Romania

[2]Chemical and Biochemical Engineering Department, National University of Science and Technology POLITEHNICA Bucharest, 1–7 Gheorghe Polizu Str., 011061, Bucharest, Romania

Abstract: *In autumn 2023 the lower Danube transect (rkm 111.5-435) was profiled, including the Mila 41, Mila 52 and Mila 64-67 delta sections, with three lateral samples per section. NOx-N ranged from 0.19 to 0.42 mg L^{-1} (mean 0. 31 mg L^{-1}), PO_4-P from 0.20 to 0.59 mg L^{-1} (mean 0.28 mg L^{-1}), and chlorophyll-a from 9.1 to 35.5 µg L^{-1} (median 14.9 µg L^{-1}). Correlations between chlorophyll-a and nutrients were weak, and adjusting for pH, total suspended solids further weakened these relationships, indicating that light limitation and hydromorphological setting are also key drivers. The conclusion emphasizes the need for an integrated monitoring system that includes nutrients and physico-chemical parameters to properly assess water quality in the lower Danube basin.*

Key words: chlorophyll-a, nutrients, phytoplankton

Introduction: Understanding how nutrient concentrations relate to chlorophyll-a along large river systems such as the Danube is essential for evaluating eutrophication and ecosystem functioning. During autumn 2023, we profiled the Romanian Lower Danube from downstream to upstream, beginning at km 111.5 (Isaccea) and extending to rkm 435 (Oltenița), with deltaic references from Mila 41 (Chilia Veche) through Mila 52 (Ceatal Izmail) to Mile 64–67 (Reni). At each georeferenced cross-section, we sampled three lateral positions across the channel to capture both longitudinal and cross-channel variability in chlorophyll-a and nutrients under autumn, generally well-mixed conditions.

Experimental part: Surface water samples (0–0.5 m depth) were collected at each cross-sectional position. Onboard the research vessel, concentrations of NOx–N (NO_2–N + NO_3–N) and PO_4–P were determined using a Hach DR 200 spectrophotometer, expressed in elemental notation and subsequently used to calculate molar N:P ratios. Chlorophyll-a was retained on cellulose membrane filters, extracted with 90% acetone, and quantified spectrophotometrically in the laboratory using a PerkinElmer UV–Vis instrument. In addition, in situ measurements of pH, electrical conductivity (CND), total suspended solids (TSS), dissolved oxygen (DO), and precise georeferenced positions were recorded for each sampling point.

Results and discussions: Along the Isaccea–Brăila/Galați–Călărași/Fetești–Oltenița transect, chlorophyll-a concentrations ranged from 9.1 to 35.5 µg/L (median 14.9 µg/L), indicating low to moderate phytoplankton biomass during the autumn period. Nitrate concentrations varied between 0.19 and 0.42 mg/L, while phosphate ranged from 0.20 to 0.59 mg/L (median 0.28 mg/L). The molar N:P ratio was between 1.1 and 4.0 (median 2.5). Correlations between chlorophyll-a and nutrient concentrations were weak to moderate, and further decreased when pH, electrical conductivity, and total suspended solids were considered. These results suggest that light availability and hydromorphological conditions exert a stronger influence on phytoplankton dynamics than nutrient levels alone in this lower Danube reach.

Conclusions: The autumn 2023 field campaign across rkm 111.5 to rkm 435 and Mila 41–67 shows that nutrient availability alone does not explain chlorophyll-a variability. Light limitation together with hydromorphological setting emerges as a co-driver of phytoplankton dynamics. These findings highlight the importance of integrating optical and hydrological parameters in assessing and managing the ecological status of the Lower Danube.

Acknowledgements: The research was financed by the Ministry of Research and Innovation - PN 23 30 01 03: “Improvement of the monitoring program of the Romanian Black Sea shelf to enhance the capacity for assessing and predicting the impact of multiple stressors on marine ecosystem services” and carried out through PN 23 30 03 03: “Optimizing the sustainable management of natural resources, increasing water security and the resilience of ecosystems in the lower Danube basin, affected by climate change and human interventions”.

AUTHORS INDEX

A	Pages
Abdelkafi Slim	23
Abdulazez Israa F.	161
Ahmed Shaalan Bdaiwi	142
Akca Mine	150
Albulescu Mihai	81, 122
Aldrigo Martino	187
Alexa Irina-Claudia	209
Alexandru Mioara	185
Altan Eray	146
Ameer Al Jaseem	173
Amroudine Moussa	118
Andronescu Ecaterina	174
Ariton Irina Maria	199
Aruș Vasilica-Alisa	225
Asoltanei A.M.	176
Ateş İsmail	154
Avcı Tubanur	158
Avram Lazăr	69
Aziam Rachid	206

B	
Baciu Ionela Otilia	212
Bădică Petre	181, 183
Bădulescu Sabina Cristiana	181
Bălănucă Brînduşa	207
Banciu Adela	148, 164
Banu Ionuţ	38, 199
Barna Alin-Andrei	115
Barylyak A.	167
Bărbulescu Andrei	71
Bârsan Doru	71
Baykara Dilruba	150
Berbecaru Andrei	134
Bingöl Ayşe Betül	159
Biró Levente	99

L	Pages
Lăcătuş A.M.	221
Lavric Roxana	170
Lavric Vasile	75, 77, 83, 224, 230
Lazăr Liliana	34
Lazău Carmen	125
Letelier-Gord Carlos Octavio	227
Liciu Eduard	165
Lisa Cătălin	67
Lisa Gabriela	65
Loridant Stéphane	111
Løes Anne-Kristin	227
Lungu (Ioniţă) Florina	95
Lungu Ionuţ	71
Lupaşcu Naliana	230

M	
Maganu Maria	142
Maior Ioana	195, 219
Mămăligă Ioan	34, 177
Manolache Andreea	38
Manolache Fulvia	207
Marcati Alain	25, 56, 106
Marcu Ioan-Cezar	111
Marin Florian	198
Marinaş Ioana-Cristina	142
Marinescu Maria	176
Mateescu Ciprian-Ştefan	165
Matei Elena	135, 170
Menaa Bouthaina	23
Meng Jun	191
Michaud Philippe	23, 27, 106, 119, 201
Miclăuş Adina-Lucreţia	49
Mihai Marcela	47
Mihalache Mihaela-Liliana	116
Mihalcea Alina	63

Bleotu Coralia 13
Bobitsk Yaroslav 167
Bodescu Adrian G. 41, 45
Bogdan Florin 81, 122
Boscencu Rica 183
Botoran Oana Romina 135
Botta Oana-Daciana 166
Bran Elena Petronela 207
Bratu Aurelia 115
Brănescu Dumitriana-Roberta-Marina 61
Brehar Marius A. 97
Brettfeld Eliza-Gabriela 193
Brezoiu Ana-Maria 38, 196
Brîncoveanu Oana 148, 152, 185, 187
Bubueanu Corina 219
Bucătăriu Florin 47
Bulgariu L. 217
Busuioc Cristina 164, 166, 169, 211

C

Cabell Joshua 223
Călinescu Ioan 15, 191, 202
Cantaragiu Claudia Ana Maria 180
Capcanari Tatiana 201, 205
Căproiu Miron Teodor 141
Casarica Angela 219
Casariu Florina 75, 77
Cauacean Radu 97
Cebotaru Nicolae 97
Celik Ali Alparslan 117
Çeltikci Şimal 154
Cesur Sumeyye 117, 158
Château T. 51
Chelmuş Vlad-Iulian 63
Chiciudean Tudor M. 97
Chipurici Petre 113
Chira Nicoleta-Aurelia 115, 212
Chiriac Anita Laura 124
Mihaly Norbert B. 97
Mihăiescu Dan Eduard 13, 182
Mihăilă Laurenţiu-Constantin 65
Mirilă Diana 179, 180
Mitran Raul A. 186
Mitrică Adrian-Marian 197
Mocanu Alexandra 91, 149, 153, 186, 188
Mocanu Andreea L. 208
Moghaddasi Mohammad 156
Moldovan Andreea 188
Moloşag Ailin 227
Moraru Teodora 63
Moşneguţu Emilian 180
Motelică Ludmila 13, 129, 133, 138, 172, 175
Moţ Andrei 227
Muntean Claudia I. 21, 43, 89
Muntianu Gabriela 180
Muslu Meryem 156
Mustăţea Gabriel 208
Muşat Viorica 140

N

Nacu Viorel 13, 175
Neagu Ana Lorena 125
Neagu Răzvan 176
Nedeff Florin 179
Nedelcu Andrei-Silviu 165
Nedelcu L. 170
Negrilă Cătălin 111
Ngo T. N. 51
Nichitoi Andreea 227
Nicoară Adrian-Ionuţ 211
Nicolae Cristian 174
Niculae Andrei Laurenţiu 114
Niculescu Florentina 135
Niculescu Ilie AnaMaria 181
Nicuţă Daniela 213
Nistor Ileana Denisa 179, 180, 229

Chiriac Radu 113
Chiriţă Andrei I. 130
Chisega Negrilă Ciprian-Gabriel 191
Chiș Timur-Vasile 53, 69, 71, 73, 75, 77, 112
Christophe Gwendoline 27, 118
Cieniek B. 167
Çiftçi Fatih 159
Ciobanu Adela Dana 144
Ciobotaru Ioana-Alina 194, 215
Ciocîrlan Oana 137
Cioroiu Gabriel-Marius 36
Ciortan Gherghina 107
Ciucure Corina Teodora 135, 197
Ciufu Alina Georgiana 145
Codreanu (Manea) Ana-Maria Nicoleta 206
Cojocari Alexandrina 201
Cojocaru Anca 194, 215
Coman Andrei 59
Coman Dumitru 34
Coman George 134
Coman Mădălin Vasile 128
Comănescu Brînduş 134
Condeiu Cristian 107
Constantin Andreea Adelina 135, 197
Constantinescu Şerban 18
Cormoş Ana-Maria 99
Cornet Jean-François 26
Covaliov Eugenia 201, 205
Crăciun Alexandra-Ioana 37
Crăciun Mihaela Emanuela 222
Cristea Diana-Ioana 219
Cristea Doru-Daniel 164
Cristea Vasile-Mircea 41, 45, 49
Cui Zhonghua 190
Curteanu Silvia 59, 61

D

Nmila Rachid 201

O

Odabaşi 160 160
Oktay Büşra 156, 160, 162
Oprea Ovidiu 13, 129, 133, 138, 172, 175
Orbeci Cristina 227
Ozbolat Ibrahim Tarik 156
Ozunu Alexandru 37, 145, 191

P

Papa Florica 111
Pârvulescu Oana Cristina 38, 53, 101, 216, 226, 227
Patrichi Claudia Ana Maria 146
Patriciu Oana-Irina 211, 213
Păvăloiu Ramona-Daniela 142, 223
Peghaire Elodie 119
Pencea Ion 135
Petcu Ionela-Cristina 149
Petraş Laura Elisabeta 43, 89
Petreanu Irina 198
Petrila Larisa-Maria 47
Petrişor Gabriela 13
Pierre Guillaume 27, 119, 201
Pintilie Lucia 142
Platon Nicoleta 229
Popa Claudia Valentina 176, 218
Popa Ioana 206
Popa Iolanda 75, 77, 83
Popa Ionuţ-Alexandru 53
Popescu Diana-Mihaela 176, 218
Popescu Grațiela Elena 226
Popescu Ionel 111
Popescu Roxana Cristina 149
Popovici Violina 205, 209
Postelnicescu Paula 93, 103
Poteraş Beatrice C. 207

Damian Celina 185
Danilova Valeria 34
Dascălu Andrei 178
Dauchet Jérémi 26
Dănilă George-Mădălin 152
Dărăban Romina G. 41, 45
Deleanu Iuliana Mihaela 53, 87, 91, 142, 211
Demostene Nicoleta-Oana 39, 87
Diacon Aurel 152, 164, 185, 187
Diaconu Ioana 101
Diculescu Victor-Constantin 166
Dimian C. Alexandre 5
Dinu Livia A. 185
Djellabi Ridha 32
Dobre Tănase 11, 39, 43, 53, 87, 89, 112, 130, 193, 223
Dobrinaş Simona 220
Doğan Canan 154, 158
Dolete Claudiu 79
Donise Andreea Cristina 222
Doroftei Raluca Florenţa 178
Dragomir Mihai 164
Drăghici Constantin 141
Drăgoi Cudalbeanu Mihaela 214
Drăgoi E. N. 176
Drăguţ Natalia 13
Dubessay Pascal 23, 27, 118
Dumitrescu Anca Mădălina 103
Dumitrescu Rucsandra 13
Duţă Elena-Alexandra 194

E

Emilian Roman 219
Enăşcuţă Cristina-Emanuela 191
Enculescu I. 169
Ene Manuela Diana 181, 183
Enescu Alessia-Ioana 211
Essid Adib 25, 51, 104

Predescu Cristian 135
Pşenovschi Grigore 192
Purcăreanu Bogdan 182
Purghel Ioana 79
Puşcaşu Doru Vladimir 19

R

Radu Oxana 205, 209
Raduly Monica Florentina 174
Rădiţoiu Alina 174
Rădiţoiu Valentin 174
Raiciu Anca Daniela 29
Reddad El Moznine 201
Reyhanoglu Melek Beyza 118
Romaniţan Cosmin 153
Roşca Anca M. 206
Roșu Ana-Maria 179, 180
Rotariu Traian 188
Rotaru Gabriela-Alexandra 167
Rusen Edina 153, 186, 188
Rusu Paula 67

S

Saeed Farqad Rasheed 143
Salifoglou Athanasios 227
Sandru Claudia 198
Sandu Teodor 125
Săpunaru Olga V. 87, 131
Saraç Ömer Faruk 155
Sârbu Andrei 125
Scrieciu Albert 230
Secară Cristina-Anca 176, 218
Secu Corina 135
Secu Mihail 135
Secula Marius S. 177
Serafim Andrada 149
Sha'at Fawzia 142, 223

F

Fediuc Florentina 226
Fendri Imen 23
Ficai Anton 13, 128, 132, 171, 174, 181
Ficai Denisa 13, 128, 132, 171, 174
Fierăscu Irina 128, 132
Fierăscu Radu Claudiu 128, 132
Fînaru Adriana-Luminiţa 207, 209
Flahaut Thomas 118
Florea Daniela 226
Florea Mihai Alexandru 181, 183
Florescu Teodor-Mihai 219
Fodor Ciprian 219
Fodor Mariana 219
Fontaine Jean-Pierre 104
Fontanille Pierre 201
Forano Claude 201
Froidevaux Rénato 47
Frone Adriana 173
Fulgheci Ana-Maria 171

G

Gaboreanu Mădălina-Diana 142
Gardarin Christine 201
Gaspar Răzvan 73
Gavrilă Adina Ionela 38, 113, 138, 206, 207, 208
Gavrilă Ana Mihaela 125, 188
Gaume Léa 119
Geană Elisabeta-Irina 136, 198
Georgescu Ana-Maria 179, 180, 229
Georgescu Maria 19
Ghosh Sougata 9
Ginga Alexandra 149
Glăvan Dragoş 138
Grigore R. 170
Grigoroşcuţă Mihai Alexandru 182

Silion Mihaela 47, 179
Sima Sergiu 138
Simedrea Bianca 87
Şişinea Aurelian 81, 123
Soceanu Alina 224
Spoială Angela 13, 133
Stan Liviu-Constantin 36
Stănescu Paul 138
State (Roşoiu) Sabrina-Patricia 149, 153
Stavarache Cristina Elena 116
Ştefan Daniela Simina 95, 127, 210
Steflea Sorin 75, 77, 83
Sterpu Ancaelena Eliza 131
Stoica Bianca Elena 125
Stoica Marian 219
Stoicescu Maria 79, 83, 85
Stroe Corina A. 208
Suhaianu Vladimir 218
Sulutaş Rabia 159
Surdu Vasile-Adrian 121

T

Tanasa Radu-Iulian 176
Tănase Florin-Cristian 197
Tauleigne Blandine 25, 56
Tekin Şilan 147
Teodorescu (Diaconescu) Georgeta 127
Teuşdea Alin 229
Timiş Andrei L. 135
Timiş Elisabeta-Cristina 49, 97
Tîrpan Doiniţa-Roxana 36, 146, 181
Toader Gabriela 153, 165, 186, 188
Tociu Mihaela 116, 208, 216
Todaşcă Cristina 207
Toma Emilia-Ioana 195
Tomescu Teodora 149
Tone Mihai 91

Gros Fabrice 26
Grosu Luminiţa 211, 213
Guez Jean-Sébastien 25, 51
Gündüz Oğuzhan 147, 155, 159
Güneş Şevval 155, 159
Guran Cosmin 113
György Romuald 121, 200

H

Hachicha Rihab 23
Halima Rchid 201
Hou Xiaoyang 27
Hussein Fawzi Hussein 143
Hussein Murad Majid 143

I

Iacob-Tudose Eugenia T. 177
Iancu Daniel 69
Iancu Petrica 39
Ibtissam Sabir 201
Ion Violeta Alexandra 201, 216, 227
Ionete Roxana Elena 136, 198
Ionescu Lucia-Elena 176
Ioniţă Daniela 179
Iordache Tanţa-Verona 125
Iordănescu Sergiu 188
Iorga Călin 69
Irimia Claudia 219
Isopencu Gabriela 91, 138, 153
Isopescu D.N. 177
Isopescu Raluca 93
Ivan Ștefan-Bogdan 111

J

Jian Mariana 13, 175
Jidveian Roxana 101
Jinga Sorin Ion 215

K

Topală Sorina Laura 101
Trică Bogdan 188
Trifan Andreea 165
Truşcă Roxana Doina 13, 129, 133, 172, 175
Tulyaganov Dilshat 147

U

Uncu Cristina 172
Ungureanu Camelia 63
Ungureanu Elena L. 208
Ursu Alina-Violeta 25, 104, 106, 119, 201
Üstündağ Cem Bulent 156, 160, 162
Ülker Yusuf 159

V

Vartolomei Nicoleta 229
Vărăşteanu Pericle 186
Vasile Dan-Adrian 13
Vasilescu Estera 36
Vasiliu Dan 230
Vereş-Dănciuţ Thomas 49
Vial Christophe 25, 51, 56, 104, 106, 201
Vîlcică Alexandru-Cristian 36
Vînătoru Mircea 15
Vîrtopeanu Mihai 85
Vizitiu (Bercea) Georgiana Irina 224
Vlăsceanu George 149
Vourc'h Thomas 26

Z

Zaharia Anamaria 125
Zaim Soumia 201
Zanov Kliment 153
Zorcă Andra-Gabriela 215
Zorilă Florina L. 186

Y

Yanikoglu Reyhan 156
Yıldız Fatih Mehmet 159

Karakurt Esin Şahsenem 160
Kim Lidia 210
Kisała Joanna 168
Kirim Tuğba 160
Kose Alpay 162
Koyuncu Ayşe Ceren Çalıkoğlu 155
Krzemiński P. 168
Kuncser Andrei 184
Kus-Liśkiewicz M. 168

W

Wojnarowska-Nowak R. 168

SPONSORS

Ludan Engineering

https://ludan-engineering.com/about-us/

JESCO

https://www.fresh-air.ro

OCON ECORISC

https://oconecorisc.ro/

SC

Chem.Eng. Free Lancer C.Serban

MERCK

https://www.merckgroup.com/ro-ro/company

Metrohm Romania

https://www.metrohm.com/ro_ro.html

CHEMCO TRADE

Highest class chemicals

https://chemco.ro

Compact Industrial

https://www.compact-industrial.ro/

emas

https://www.e-mas.eu

ALBA ALUMINIU

ALUMINIUM PIGMENTS

https://www.albaaluminiu.ro

edibon

https://www.edibon.com/en/

SUPPORT INSTITUTIONS

Romanian Chemical Engineering Society
132 Calea Griviţei, Building A, Room A212, Bucharest
www.sicr.ro

Romanian Chemistry Society

Faculty of Chemical Engineering and Biotechnologies

Department of Chemical and Biochemical Engineering

Academy of Technical Sciences – Chemical Engineering Section

National University of Science and Technology POLITEHNICA Bucharest

Department of Science and Engineering of Oxide Materials and Nanomaterials