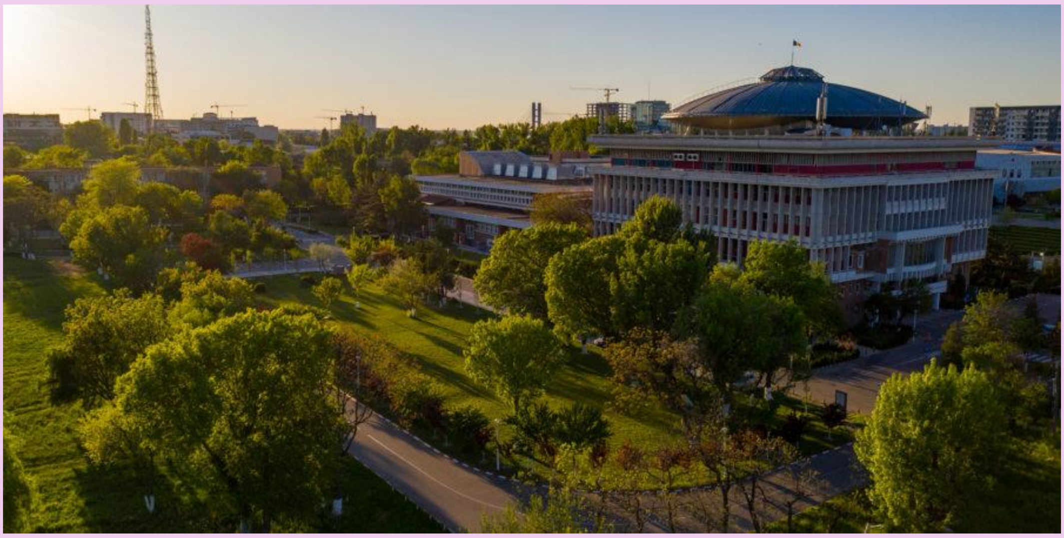

SICHEM 2024

BOOK OF ABSTRACTS

11 – 12 April 2024

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
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BOOK OF ABSTRACTS

SICHEM – 2024

Plenary

PL01 FROM WHERE TO WHERE IN CHEMICAL ENGINEERING BY PARADIGMS

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Abstract: *Chemical Engineering bible roots, middle ages roots respectively the roots referring to to the first industrial revolution was presented as precursors of the first paradigm for specialists instruction in chemical fabrications. The transport phenomena paradigm is detailed presented because it is the basis of paradigms issues after 1990. A scheme showing the link between chemical engineering paradigms and curricula dynamics is considered. An idea on haw must to be the chemical engineering curricula after the Intensive Processes and Artificial Intelligence Paradigm are given*

Key words: Chemical Engineering Roots, Paradigms, Transport Phenomena, Amundson Report, Intensive Chemical Engineering, Artificial Intelligence

Introduction: Chemical engineering has always been a science and profession that has evolved step by step, reaching today a curricular structure that must consider its development on intensive paths with strong artificial intelligence support [1]. The work reviews the most important aspects related to this evolution.

Chemical Engineering Evolution: The paper opening shows the bible roots of this science and give some date respect to this science importance for development of the ancient world. Looking back on the chemical engineering road will find their strong roots in medieval alchemy. The basic three alchemists dreams (Diderot Encyclopedia) which sought to obtain i) the creation of the fabled philosopher's stone, ii) the ability to transmute base metals into noble metals (gold or silver), iii) the development of an elixir of life for youth and longevity, can be today three major directions in which chemical engineering can go on. The processes Leblanc and Solvay for industrial sodium carbonate production and the processes (distillation and others) characterizing the beginnings of petroleum industry are considered as roots of modern chemical engineering science. Now at the finish of 19th and starting of 20th century did time for chemical engineering to gather the results, to establish their theoretical explanation and to generalize them. Such have been created the conditions for her enrolling by specialists training in the triangle education-research-production. It is known that the name of chemical engineer began to be used since 1880 as it is known that the chemical engineer of this time was in fact a mechanical engineer by training with a very a good practical knowledge of applied chemistry (chemical engineering). George Davis, an inspector in the production of England alkaline factory, hold in 1887 a total of 12

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lectures with chemical engineering specifics and titles at the Technical School in Manchester.

Chemical Engineering Paradigms: Recognizing the paradigm as a philosophical and theoretical framework of a scientific school or discipline within which theories, laws, and generalizations and the experiments performed in support of them are formulated, and looking with eyes to the passed time, we easy find for chemical engineering discipline three paradigms: the first paradigm called *Unit Operations paradigm* (1923-1960); a second paradigm called *paradigm of Transfer Phenomena* (1960 -1998), and that the third paradigm accepted as paradigm of *Process Engineering as Innovation, Design and Manufacture of High Technology Products* (1998 -2010). In a different time period, the chemical engineer training was done after one or other of these paradigms. Therefore, a succinct characterization of these paradigms is of interest. An important attention is given to the Amundson report [2] (1988) because it recommend an alliance of industry, academia and government to invest in the future of chemical engineering, which promises to serve society by: 1) Starting of New Technologies that would improve the quality of life with new products through: a) biotechnology and biomedicine; b) electronic, photonic, and recording materials and devices; c) micro structured materials; 2) Maintaining Leadership in Established Technologies and particularly in: a) in-situ processing of energy and mineral resources; b) liquid fuels for the future; 3) Protecting and Improving the Environment and Health by: a) responsible management of hazardous substances; b) protection from sudden plant disasters; 4) Developing Systematic Knowledge and Generic Tools that would be used in all three previous areas, and particularly in: a) advanced computation methods and process control; b) surface and interfacial engineering. The Amundson report keeps today their actuality. This paper shows this by presenting and commenting on some basic directions in which will be the future development of chemical engineering. The Amundson report announces that the time has come for a new organization to come up with a new paradigm in the training of chemical engineers. The *Chemical Product Engineering Paradigm* or with other name Process Engineering as Innovation, Design and Manufacture of High Technology Products, announced by the Amundson report and theoretically introduced with the book of Cuessler and Moggridge [3], must be seen in the context of the industrial products market, where their diversity (in many cases with similar properties and with the same use) has a huge increase, a fact that requires a competition of very strong market among industrial producers. Apparently beyond what is specific in the training of the chemical engineer, this paradigm requires that we add a strong market (marketing) component to this training. Things are not quite like that because the training of the chemical engineer must be oriented in such a way that it responds to four big steps imposed by the development of an easy marketable chemical product: (1) identification of customer needs, (2) generation of ideas to satisfy these needs, (3) choosing between ideas and (4) manufacturing the product. Only the first stage is related to market research [4], the next two have in them experimental and conceptual research or molecular modeling of the process, the fourth being that of the chemical processing process, where several requirements must be answered: (1) what kind of process will be used (batch process versus continuous process), (2) how process inputs and outputs are characterized (balance sheets, integrated flowsheet, etc.), (3) what reactors and recycles are used and (4) how are the separations carried out in the process and how are they integrated into the reaction and recycling systems? A fourth paradigm of interest in chemical engineer training would be the *Paradigm of Sustainable Chemical Engineering*. This paradigm [5] is based on the recognition of the time limitation of resources, the requirement of inter- and transgenerational equity within human society and, above all, the need to preserve the life that supports natural systems. Lately, as a consequence of accentuated increasingly coupling of bioengineering, biotechnology and biochemistry with chemical engineering, there is a trend towards a new paradigm, called the *Paradigm of Chemical Biotechnology,* which is gaining ground in the training of the chemical engineer. Biotechnology is biologically based ecological engineering with multiple uses, in the evolution of which chemical engineering methods can bring success ever closer. Biology, biochemistry, and biotechnology have been introduced in many countries to complement the curricula of chemical engineers. Starting with 2010, with emphasis after 2020, the orientation in chemical engineering is for intensive processes analyzed, conceptually tested and designed with the support of artificial intelligence. Or this implies the transition to a new paradigm in the training of chemical engineers. This would be Chemical Engineering through *Intensive Processes and Artificial Intelligence.* In this sense, we note the concentration of process intensification [6,7] at the level of fundamental principles (i) maximizing the effectiveness of intra- and intermolecular events in the process, ii) all molecules the same experience in the process, iii) optimizing the driving forces in the process at any scale and maximizing the surfaces on which they act on, iv), maximizing the synergistic effects of the processes, including the secondary ones) which cannot progress without adapting to them of artificial intelligence principles [8.9]. brought to the current forms of expression of process software as human-machine interaction.

Conclusion: The justification of a new paradigm in chemical engineering appeals to the identification of the actual state of the scientific and industrial requirements brought to the first and then of the other paradigms associated with the discipline. Even if it was not expressly stated, it can be deduced that in chemical engineering the main paradigms have developed, as in all engineering sciences, in that the new one takes important from the old one, often by generalization, and then updates it to the new current reality or to near future estimated through as much and deeper mathematical modeling. The parallel paradigms, as is here the case of *Paradigm of*

Sustainable Chemical Engineering and *Paradigm of Chemical Biotechnology*, come to emphasize aspects of the paradigm with which they are face to face (*Chemical Product Engineering Paradigm* here).

References:

[1] Dobre T., Stoica Anicuta., *Mass Transfer Enhancement*, Electra Press, Bucharest, 20017.

[2] * * * Committee on Chemical Engineering Frontiers: *Research Needs and Opportunities (Amundson Report)*, National Research Council of United State, ISBN: 0-309-55519-1, 232 pages, 1988, New York

[3] Cussler E. L., Moggridge D. G., *Chemical Product Design*, Cambridge University Press, First. Edition 2001

[4] Hill M., *Chemical Product Engineering-Third Paradigm*, Computers and Chemical Engineering, 33, (2009), 947–953.

[5] Narodoslawsky M., *Chemical Engineering in a Sustainable Economy.* Chem. Eng. Res. Desgn. 91, (2013), 2021–2028.

[6] Boodhoo, K., Harvey, A., (Eds), Process Intensification for Green Chemistry: Engineering Solutions for Sustainable Chemical Processing, John Wiley & Sons, 2013

[7] Gerven V.T., Stankiewicz A., Structure, Energy, Synergy, Time - The Fundamentals of Process Intensification, Ind. Eng. Chem. Res., 48, 2465–2474, 2009

[8] Nilsson N., Principles of Artificial Intelligence, Tioga Press, Palo Alto, California, 1980

[9] Quantrille E. Th., Y. A. Liu A. Y., Artificial Intelligence in Chemical Engineering, Academic Press, 2012

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 - IE 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.

PL02 ARTIFICIAL INTELLIGENCE FOR CHEMICAL ENGINEERING

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Abstract: *An introduction in the use of artificial intelligence in chemical engineering was performed using the flame spray pyrolysis process as an example.*

Key words: Artificial Intelligence, Chemical Engineering, Flame Spray Pyrolysis

Introduction: Artificial intelligence (AI) is a component of computer science concerned with designing programs that simulate human intelligence [1]. The application of AI to chemical engineering builds upon the success of expert systems and neural networks that have been used for a long time in this research and design area. The present paper emphasizes the most recent developments and trends in the AI field.

Experimental and/or Modelling: Recent developments in artificial intelligence (AI) have turned computers into "assistants" capable of guiding research and development in a meaningful way [2]. In this conference, the concept of "intelligent software" is presented. The software includes elements of AI such as machine learning, computer vision and natural language processing. The value of the approach is illustrated using real-time optimization of the Flame Spray Pyrolysis synthesis process. After proper training, the intelligent software becomes a trusted partner of the technologist in monitoring the stability of the flame and adjusting control parameters – in real-time – to address off normal conditions [3]. In addition, a discussion about the current and future applications of AI in chemical engineering demonstrates that the human-AI partnership is changing science and technology for the better.

Conclusions: It has been shown how one can use the computer software as an assistant in guiding chemical engineering research and development. The flame spray pyrolysis process was used as an example of successful human-computer partnership.

References:

[1] Quantrille E. Th., Y. A. Liu A. Y., *Artificial Intelligence in Chemical Engineering*, Academic Press, 2012

[2] G. Sivaraman, M. Stan et al. Phys. Rev. Let. 126 (2021) 156002

[3] J. Pan, M. Stan et al., Int. J. Adv. Manuf. Tech. 114 (2021) 2215

About the author: Dr. Marius Stan is a Senior Scientist and Leader of Intelligent Materials Design in the Applied Materials Division at Argonne National Laboratory. He is also a Senior Fellow at the University of Chicago and Northwestern University. Marius and his team use artificial intelligence (AI) and high-performance, multi-scale computer simulations to understand and predict physical and chemical properties of multi-component metals and ceramics. The applications include energy production (nuclear fuels and reactor materials), energy storage (batteries) and electronics. The team also uses AI to optimize complex processes for manufacturing applications such as 3-D printing and flame spray pyrolysis. Marius has extensively published in scientific literature, holds several patents, and is currently writing a book on modeling and simulation. He is also an author of short stories and poetry. Some will recognize him as an actor, portraying Bogdan in the award-winning TV series Breaking Bad.

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PL03 ADVANCED CERAMIC POWDERS OBTAINED VIA HOST GUEST POLYMERIZATION

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Abstract: *The work presents the results obtained during the studies about the obtaining of ceramic powders starting from mesoporous inorganic hosts in which took place the radical polymerization of a vinyl monomer, the obtained polymer nanocomposites being converted by thermal processing, first in carbon nanocomposites and latter on in silicon nitride. silicon carbide or titanium nitride, depending on the inorganic host: silica or titania and on the atmosphere of the high temperature reaction (Nitrogen or Argon.)*

Key words: ceramic powders, polymer nanocomposites, silicon nitride, silicon carbide, titanium nitride, host guest polymerization

Introduction: The silicon nitride, silicon carbide and titanium nitride are raw materials for structural ceramics. Various methods can be used in order to synthesize them. For instance, best quality Si_3N_4 or TiN, can be prepared by a carbothermal nitridation reaction [1] :

$$3\ SiO_2\,(s) + 6\ C\ (s) + 2\ N_2\,(g) \rightarrow Si_3N_4\,(s) + 6\ CO\ (g) \qquad (1)$$

$$2\ TiO_2\,(s) + 4\ C\ (s) + N_2\,(g) \rightarrow 2\ TiN\,(s) + 4\ CO\ (g) \qquad (2)$$

SiC can be prepared by a similar reaction with that in equation 1, but in Argon, instead of Nitrogen. For reactions (1) and (2), involving two solids and a gas, the intimate mixtures of the solids is essential. These mixtures can be obtained by filling the carbon nanotubes with silica or titania or by the polymerization of a vinyl monomer in sepiolite hallow fibers, with subsequent carbonization of the polymer [2,3]. The present work describes the results obtained for another choice: the host guest polymerization of vinyl monomers in mesoporous silica or titania, followed by the carbonization of polymers.

Experimental: *Reagents:* acrylonitrile (AN) p.a (Merck) as monomer, which was distilled for the elimination of the inhibitor, azoizobutirodinitrile (AIBN) p.a (Merck) as initiator, mesoporous silica or mesoporous titania, both produced in lab, the first by acid attack of serpentinite and the second by sol-gel; *Polymer nanocomposites obtaining* took place at 60-70ºC in inert atmosphere*: Carbon*

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nanocomposites obtaining took place by thermal treatments in the range 200-1000°C. *Si_3N_4, SiC and TiN* were obtained by carbothermal reaction in N_2 or Ar at 1200- 1450°C.

Results and discussions: The results obtained during the studies about the preparation of the inorganic hosts, during the host guest polymerization, during the transformation of polymer nanocomposites in carbon nanocomposites and during the carbothermal synthesis are presented and discussed. For instance, in figure 1 a TEM photography of a polymer nanocomposite is presented, showing the inclusion of polymer inside the nanopores of silica and in figure 2 and 3 some XRD of a carbon nanocomposite and of a prepared Si_3N_4 are presented, the first diffractogram presenting an amorphous structure and the second diffractogram presenting the picks of α and β silicon nitride.

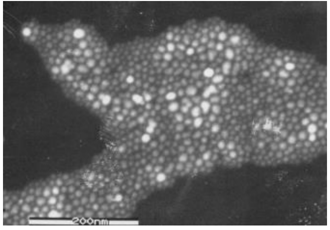

Fig.1 TEM photography of a polymer nanocomposite

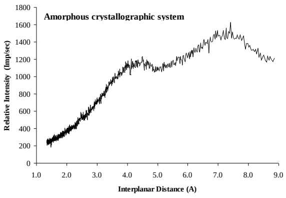

Fig.2. XRD Spectrum of a silica- carbon nanocomposite

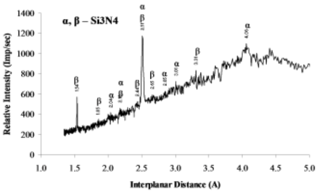

Fig.3 XRD spectrum of prepared Si_3N_4

Conclusions: Host guest polymerization of a vinyl monomer inside the mesopores of silica or titania, followed by the polymer carbonization, is an advanced method which allows the preparation of an intimate mixtures of the carbon with the inorganic host, leading to the synthesis of high quality ceramic powders.

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References:

[1] Pavarajarn V., Kimura S., J. Amer. Ceramic Soc., , 84 (8) (2001)1669-1674

[2] Gundiah G., Madhav G. V., Govindaraj A., Seikh M.M., Rao C., J. Mat. Chem., 12 (5) (2002) 1606 - 1611

[3] Kurt A.O., Davies T.J, J. Mat. Sci., 36 (24), (2001) 5895-5901,

[4] Locovei C., Chiriac A-L., Miron A., Iftimie S., Antohe V., Lazau C., Sarbu A., Dumitru A., Scientific Reports 11, (2021) 5055

PL04 ULTRASOUND AND MICROWAVES USEFUL TOOLS IN PROCESS INTENSIFICATION

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The 21st century has witnessed a growing emphasis on environmental awareness and the need for greener technologies to reduce emissions and improve energy efficiency [1].

Process intensification (PI), which focuses on enhancing material and energy efficiency, safety, and environmentally friendly processing, is recognized as a promising approach in chemical and process engineering to overcome these challenges and drive progress [2]. PI enhances energy efficiency by reducing mass and heat transfer resistances and overcoming thermodynamic limitations through integrated design and operation.

Microwaves and ultrasound are recognized as two effective methods of intensifying processes. In the laboratory of Ultramint-techologies (https://eertis.eu/errf-2300-000c-2090) there is a wide range of equipment using microwaves and ultrasounds. Many of them are unique at national level (DFR, MMM Clamp on, cuphorn for US and Labotron, respectively cavity resonance for MW). The characteristics of these equipments and the results obtained (extraction of tannins from oak bark, degradation of some toxic compounds (bisphenol) from water , etc.) will be presented.

In the second part of the conference will be presented a working methodology on the US bath that allows obtaining reproducible results and an optimal transfer of US energy from the transducer to the reactor.

References:

[1] *J.G. Segovia-Hernández, S. Hernández, E. Cossío-Vargas, and E. Sánchez-Ramírez*, "Challenges and opportunities in process intensification to achieve the UN's 2030 agenda: Goals 6, 7, 9, 12 and 13", Chemical Engineering and Processing - Process Intensification, 2023. **192**: p. 109507 10.1016/j.cep.2023.109507.

[2] *F.J. Keil*, "Process intensification", Reviews in Chemical Engineering, 2018. **34**(2): p. 135-200.

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About the author: Prof. Dr. Ing. Călinescu Ioan, has a very good expertise in the use of microwaves, ultrasound and accelerated electrons in the intensification of processes, the synthesis of metal nanoparticles, the treatment of gases and waste water, etc. Co-author of over 115 ISI papers and 15 national patents granted. It has 1158 citations in ISI Web of Science and 2319 citations in Google Scholar. PhD supervisor since 2016, 24 theses completed. Responsible for more than 20 national and international projects. He is the coordinator of a research platform dedicated to the use of ultrasound and microwaves in process intensification (https://eertis.eu/errf-2300-000c-2090).

PL05 SONOCHEMISTRY – ORIGINS AND EVOLUTION –

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Abstract: *Sonochemistry: Origins and Evolution*

Key words: Historical appearance, early stages, Romanian contributions, where is today.

Introduction: Sonochemistry, as a defined subject, has a surprisingly short history of just over 50 year and the first meeting entirely devoted to it took place in 1986 [1]. The European Society of Sonochemistry was born 40 years ago but its origins can be traced to the much earlier time of around 100 years ago [2]. This presentation will show the route by which the initial work on this branch of chemical science "SONOCHEMISTRY" evolved. We may consider now that sonochemistry is a part of general chemistry in the same way as photochemistry, electrochemistry, microwave chemistry, etc., [3].

Presentation: The very first time that the term sonochemistry was used was in 1951 by Weyl in a paper entitled "Surface structure of water and some of its physical and chemical manifestations" [4]. Before that all experiments in the field were reported as the effects of ultrasound on different media (especially water) via induced cavitation. Various contributions from the pioneers of this science will be presented, starting with the work of Marinesco [5] and ending with the latest articles published by our group here in Romania. Some of the topics which have grown and developed from sonochemistry have helped to make the authors of this presentation be acknowledged as two of the *"true pioneers"* in this area of chemistry. These topics include : environmental protection [6], food technology [7], herbal extraction [8, 9] and the synthesis of biodiesel [10, 11]. Other scientists who have made fundamental contributions to sonochemistry will also be mentioned during this presentation [10, 12-14].

Conclusions: The aim is to draw the attention of the audience to this branch of chemical sciences. It combines a knowledge of chemistry with physics and materials science. Many new discoveries have already been made and more remain to be discovered by those who engage in research and development in this exciting field of science known as sonochemistry.

References:

[1] T.J. Mason, Sonochemistry symposium at the Annual Chemical Congress of the Royal Society of Chemistry, University of Warwick, UK, 8-11 April 1986, Ultrasonics, 25 (1987) 5, https://doi.org/10.1016/0041-624X(87)90002-3.

[2] R.W. Wood, A.L. Loomis, XXXVIII. The physical and biological effects of high-frequency

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[*] Corresponding author: mircea.vinatoru@gmail.com; mircea.vinatoru@upb.ro.

sound-waves of great intensity, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 4 (1927) 417-436, 10.1080/14786440908564348.

[3] T.J. Mason, M. Vinatoru, Sonochemistry: Fundamentals and evolution, 2023.

[4] W.A. Weyl, Surface structure of water and some of its physical and chemical manifestations, Journal of Colloid Science, 6 (1951) 389-405, https://doi.org/10.1016/0095-8522(51)90011-6.

[5] M. Marinesco, J.J. Trilla, Action des ultrasons sur les plaques photographiques, Compt. Rend. Acad. Sci., 196 (1933).

[6] T.J. Mason, Sonochemistry and the environment - Providing a "green" link between chemistry, physics and engineering, Ultrasonics Sonochemistry, 14 (2007) 476-483, 10.1016/j.ultsonch.2006.10.008.

[7] M. Povey, T.J. Mason, Ultrasound in Food Processing, Blackie Academic and Professional, 1998.

[8] M. Vinatoru, M. Toma, T.J. Mason, Ultrasonically assisted extraction of bioactive principles from plants and their constituents, in: T.J. Mason (Ed.) *Advances in Sonochemistry*, JAI Press, 1999, pp. 209-248.

[9] T. Mason, M. Vinatoru, Ultrasonically assisted extraction in food processing and the challenges of integrating ultrasound into the food industry, Ultrasound in food processing: Recent advances, (2017) 329-353.

[10] C. Stavarache, M. Vinatoru, R. Nishimura, Y. Maeda, Conversion of vegetable oil to biodiesel using ultrasonic irradiation, Chemistry Letters, 32 (2003) 716-717.

[11] Y. Maeda, M. Vinatoru, Carmen-Eugenia Stavarache, K. Iwai, H. Oshige, Method for producing fatty acid alcohol esters, in: United States Patent, COSMO OIL Japan, United States Patent, 2004.

[12] T. Ando, S. Sumi, T. Kawate, J. Ichihara, T. Hanafusa, Sonochemical switching of reaction pathways in slid–liquid two-phase reactions, Journal of the Chemical Society, Chemical Communications, (1984) 439-440, 10.1039/C39840000439.

[13] J. Luche, C. Einhorn, J. Einhorn, J. Sinisterra-Gago, Organic sonochenistry: A new interpretation and its consequences, Tetrahedron Letters, 31 (1990) 4125-4128, https://doi.org/10.1016/S0040-4039(00)97559-2.

[14] M.E. Fitzgerald, V. Griffing, J. Sullivan, Chemical Effects of Ultrasonics—``Hot Spot" Chemistry, The Journal of Chemical Physics, 25 (1956) 926-933, http://dx.doi.org/10.1063/1.1743145.

Dr. Mircea Vinatoru is a Senior Scientist at Polytechnic University of Bucharest. Is having over 32 years of experience in sonochemistry. He has applied the sonochemistry to natural products extraction, biodiesel synthesis, antimicrobial fabrics hybrid technology (microwave and ultrasound together) and on leather tanning and processing.

Prof. Timothy J. Mason is Emeritus professor at Coventry University (UK) having over 40 years' experience in sonochemistry. He made major contribution to this science and was the first president of the European Society of Sonochemistry, still active nowadays. He was the initiator and editor of a new journal: Ultrasonics Sonochemistry, with an impact factor 8.4 in 2023.

PL06 MICROBIAL BIOPOLYMERS RESEARCH IN THE NATIONAL INSTITUTE OF CHEMICAL PHARMACEUTICAL RESEARCH AND DEVELOPMENT-ICCF

Misu Moscovici[1,*]

[1]National Institute of Chemical Pharmaceutical research and Development-ICCF

Abstract: *Microbial biopolymers research in the National Institute of Chemical Pharmaceutical Research and Development-ICCF*

Key words: Polysaccharides, Polyhydroxyalkanoates, Bacterial Cellulose

Introduction: Thanks to their special advantages: renewable resources origin, biodegradable, biocompatible, non-toxic, non-immunogenic, non-mutagenic, some microbial biopolymers were constantly in the spotlight of the research fields of the institute, becoming a traditional direction since the1970’s, favored by the existence of its own collection of industrial importance microorganisms (CMII). Three important classes of such biopolymers due to their unique properties and large domains of developing applications have been of interest: exopolysaccharides, polyhydroxyalkanoates and bacterial cellulose. This presentation follows the chronological order of their study in the institute.

Exopolysaccharides. This class of biopolymers is represented by polymers of monosaccharide units, mostly hexoses, connected by glycosidic bonds, secreted extracellularly by their producing microorganisms.

Pullulan polysaccharide

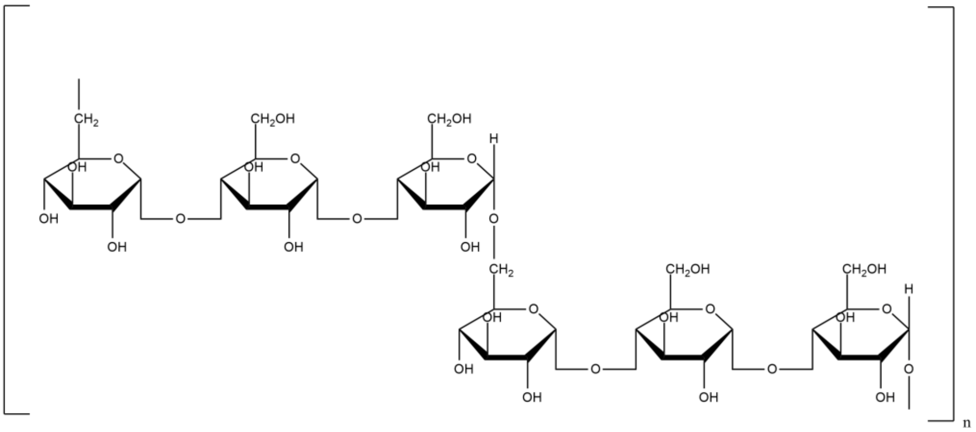

Figure 1. Structure of pullulan

This linear monosaccharide of maltotriose units (Figure 1) shows unique properties of forming water soluble oxygen impermeable, elastic, transparent, edible, tasteless, odorless films and folies, easy moldable, with an easily chemically modifying

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structure; its commercial production was launched in 1976 by an almost yet unique Japanese producer, has been in the market since 1982 [1], but its potential applications are in development until today [2].

Started already in the 1970's, ICCF research achieved remarkable results since 1990, when original fast-producing mutant strains of the yeast-like *Aureobasidium pullulans* were obtained, with high volumetric productivity and product final concentrations in batch and fed-batch fermentation on microfermenter and pilot scale were possible by biochemical engineering studies.

Other microbial polysaccharides have been developed: of curdlan, xanthan-type, as well as original ones, with interesting monosaccharide compositions produced by nature isolated bacterial strains (e.g. produced by *Klebsiella oxytoca*, and a recent one, rhizoban, produced by a *Rhizobium radiobacter* strain.

A downstream processing technology, including ultrafiltration membranes was developed, leading to high quality products**.**

Chemical semisynthetic derivatives of pullulan, with controlled properties and potential pharmaceutical applications were developed by partnership. Nanoparticles of pullulan acetate entrapping the antitumoral 5-fluorouracil were recently prepared and studied in the institute.

Polyhydroxyalkanoates (PHA)

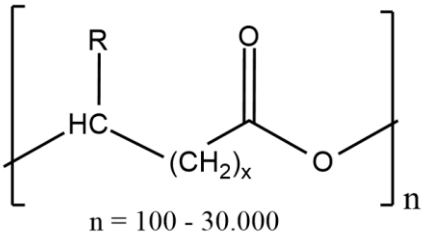

Figure 2. General structure of polyhydroxyalkanoates

They are polyesters of R-hydroxyalkanoic acids (Figure 2) differing by the monomer structure: the number of carbon atoms in the main chain and of the radical R. With similar properties to synthetic polymers, particularly polyolephins, but obtained from renewable resources and biocompatible, eco-friendly, they are increasingly considered alternatives for synthetic ones, with applications ranging from tissue engineering to packaging materials [3]. Secreted intracellularly by bacteria as carbon and energy store materials from stress by low nutrients and carbon excess, they are hydrophobic, water insoluble and should be downstream processed by solvent extraction. Two nature isolated strains of *Pseudomonas* (*putida* and *fluorescens*) were used as producers. A fed-batch procedure using *Pseudomonas putida* and C6, C8 as precursors led to the best results regarding biomass and its containing PHA, purification yield, as well as a reproducible monomer composition to an elastomer quality

Valuable composites were prepared and tested by partnership and their biodegradability was tested.

Bacterial cellulose

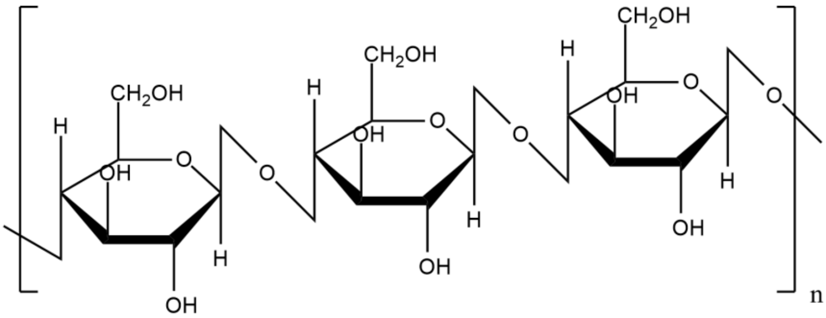

Figure 3. Structure of bacterial cellulose

A linear homopolysaccharide formed β-D-glucopyranose units linked by β-1,4 glycosidic bonds (Figure 3), bacterial cellulose is a future promising direction in cellulose development, by its important advantages: the possibility to control the product characteristics (shape, network) and yield by bioprocess parameters and the most important in applications, the bacterial synthesis results in a direct nanofiber product with very high water absorption [4]. The best results have been obtained in the institute with a collection strain of *Gluconacetobacter xylinum* (former name *Acetobacter*), in surface static conditions on a culture medium containing as carbon sources damaged fruits (apple, pears) and glycerol at 1L working volumes.The formed surface pellicle of nanocellulose was collected and purified.

The very high water holding capacity (more than 99%), forming stable hydrogels, made it an ideal material for wound healing, successfully tested on pets.

Numerous other composites were obtained in partnership.

Conclusions: Biological synthesis of microbial biopolymers and the down-stream processes to valuable products has been a traditional research topic of ICCF, achieving remarkable and original results in all the stages of the bioprocess, starting from new nature isolated strains to original aspects of the technological flowsheet and products of original composition and high quality.

Such results made possible the development of valuable chemical derivatives and composites, as well as their applications by partner institutions.

References:

[1] Singh R.S., Kaur N., Singh D., Purewal S.S., Kennedy J.F., Pullulan in pharmaceutical and cosmeceutical formulations: A review. Int. J. Biol. Macromol. 231 (2023) 123353. https://doi.org/10.1016/j.ijbiomac.2023.123353

[2] Krebs de Souza, Ghosh T., Lukhmana N., Tahiliani S.,Hoffmann T.G., Purohit S.D., Han S.S., Pullulan as a sustainable biopolymer for versatile applications: A review. Mater. Today Commun. 36 (2023) 106477. https://doi.org/10.1016/j.mtcomm.2023.106477.

[3] Behera S., Priyadarshanee M., Das V. S., Polyhydroxyalkanoates, the bioplastics of microbial origin: Properties, biochemical synthesis, and their applications. *Chemosphere* 294 (2022) 133723, https://doi.org/10.1016/j.chemosphere.2022.133723.

[4] Swingler S., Gupta A., Gibson H., Kowalczuk M., Heaselgrave W., Radecka I., Recent advances and applications of bacterial cellulose in biomedicine. Polymers 2021, 13, 412. https://doi.org/10.3390/polym13030412.

About the author: Dr. Misu Moscovici is a Senior Researcher of the Pharmaceutical Biotechnologies Department from the National Institute of Chemical Pharmaceutical R&D-ICCF Bucharest. Graduate in Organic Chemical Engineering and PhD in Chemistry-Biotechnology at The Gh. Asachi Technical University of Iasi, he worked as researcher in downstream processing of antibiotics at the ICCF-Research Centre at the Antibiotic company Iasi in 1974-1981 and since 1982, at the Institute of Chemical Pharmaceutical Research of Bucharest, in biological synthesis and downstream processing, mostly of microbial polysaccharides and enzymes. During 1994-2020 he was the general director of the institute, but during the same time he continued his R&D activity coordinating his team. He published papers, book chapters and obtained patent registrations in the field.

PL07 SCREENING, IDENTIFICATION AND IMPLEMENTATION OF POLYSACCHARIDES FROM MICROALGAE AS BIOLOGICAL AGENTS AND HYDROCOLLOIDS

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Abstract *Marine organisms are one of the most underutilized biological resources. The extreme diversity of microalgae, unicellular photosynthetic organisms that are known to produce large quantities of polysaccharides, makes them very attractive for bioprospecting and potential exploitation as commercial sources of exopolysaccharides. Indeed, exopolysaccharides from microalgae have been poorly studied compared to those from bacteria, fungi, terrestrial plants or macroalgae. A french interdisciplinary research project with approaches of biochemistry, physico-chemistry, process engineering and microbiology was conducted between 2015 and 2021. Its main objective was to increase the level of knowledge about the production of soluble polysaccharides with original structures by microalgae from marine and freshwater environments. It intended to develop the scientific background necessary for the industrial exploitation of these exopolysaccharides as hydrocolloids and/or biological active agents and to evaluate economic and environmental impacts of large-scale production. Correlations between original and published structures of exopolysaccharides and the taxonomic affiliation of microalgae producers have been highlighted for the first time. The implementation of physiological stress strategy led to accumulation of exopolysaccharides during microalgae cultivation. After their depolymerization some polysaccharides have been sucessfully tested as anti-age care and slimming agent. Other ones revealed unusual texturant properties as fluid gel behavior.*

Keywords: Exopolysaccharide, polysaccharide, microalgae, Cyanobacteria, photobioreactor

Brief Bio-sketch

Philippe Michaud, *Full Professor* of biochemistry since 2005, is head of the "4Bio" research group at the Pascal Institut, an interdisciplinary research laboratory of Clermont Auvergne University, France. 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 266 research papers and 20 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 25 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, deputy editor of Bioengineered, 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. Since 2023 he is President of the National Council of Universities for Biochemistry and Molecular biology.

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PL08 HYDROGEN GAS MASS TRANSFER IN AQUEOUS MEDIA: APPLICATION TO BIOLOGICAL METHANATION

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Pierre Fontanille, Jean-Sébastien Guez

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Abstract: *An overview of advances in the analysis of H_2 gas-liquid mass transfer is provided, with a focus on the main ways to overcome the mass transfer limitation in biological methanation.*

Key words: Hydrogen solubility, Bubbly flow, Enhancement of mass transfer

Introduction: Green hydrogen (H_2) from renewable resources is expected to become an important part of our clean and secure energy future but has not yet reached its full potential. One of the main reasons is the challenge of H_2 storage. To overcome this challenge, H_2 conversion to ammonia, methane, or formate was proposed. Formate and CH_4 can be produced from carbon dioxide (CO_2) and H_2 through biological pathways, but these gas-liquid reactions are limited by low mass transfer rate [1]. The aim of this talk is to summarize the recent advances in this field with a focus on CO_2-H_2 biomethanation.

Experimental and/or Modelling: Not only the gas-liquid mass transfer of hydrogen gas in aqueous media gas is limited by the low solubility of H_2, but classical correlations based on oxygen absorption poorly predict the volumetric mass transfer coefficient k_La for H_2. This is due to both the limited access to soluble hydrogen concentration in liquid media and to the limitations of conventional methods, such as dynamic gassing-out, which assumes that bubble size and gas hold-up are the same for H_2 and an inert gas. Thus, gas-liquid mass transfer remains poorly understood. This conference will summarize recent advances and remaining challenges in this field with an application to the enhancement of biological methanation. Perspectives based on ongoing developments, such as off-line, on-line, or in-line mass transfer rate measurements in bioreactors, in-situ microscopy coupled to artificial intelligence for bubble size and microorganism concentration, will be discussed.

Conclusions: Even though the enhancement of H_2 mass transfer rate in biological media is not fully understood, recent advances in measuring techniques, modeling tools, and bioreactor design indicate a high potential for process intensification. This is expected to be extended to other hydrogenation reactions in aqueous media in the future.

References:

[1] Jensen M. B., Ottosen L. D. M., Kofoed M. V. W., H_2 gas-liquid mass transfer: A key element in biological Power-to-Gas methanation, *Renew. Sust. Energy Rev.*, 147, (2021), 111209

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About the author: Dr. Christophe Vial is a Chemical Engineering Professor at Clermont Auvergne University in France. He is also the head of the Energy Master's Program at Polytech Clermont Engineering School. Since 2017, he has been the Deputy Director of Pascal Institute (France), an interdisciplinary research unit in engineering 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 co-authored over 120 papers and around 180 communications in congress and seminars on these topics.

PL09 UNRAVELING THE COMPLEXITY OF PHOTOREACTIVE SYSTEMS

Fabrice Gros*, Guillaume Foin, Jérémi Dauchet, Thomas Vourc'h, Jean-François Cornet

Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, F-63000
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Abstract: *Photoprocesses are very complex, to gain understanding it is necessary to combine model and devoted experiments*

Key words: Photoreactive process, modelling, experiments

Introduction: Considering the exhaustion of fossil resources and CO_2 emission rise due to their combustion, the use of solar renewable energy is evidence to cope with a constant increase of human needs for energy. This resource being naturally fluctuating, it is necessary to convert it into storable energetic vectors, the solar fuels. Their production can be carried out using photoreactive chemical systems in devoted apparatus where light absorption and reactions are supposed to occur.

Experimental and Modelling: To fully understand, the different steps involved, we developed for the systems a multiscale and predictive model that comprises four levels: i) Catalyst spectral optical properties determination which can be experimentally done or found in databases. ii) Calculation of spectral radiative properties (phase function, absorption and scattering coefficients) of the photocatalyst particle done by solving Maxwell's equations. iii) Resolution of the photon transport equation to determine luminance distribution over the entire system volume. iv) Formulation of thermokinetics coupling laws. The three last levels of this multiscale model are addressed in group, they will be illustrated by examples from our research team work [1-3].

Conclusions: The approach of our group to thoroughly describe photoreactive system is presented. It can be used in order to conceive, implement, optimize new reactors operating with solar light.

References:

[1] Supplis, C., Dauchet, J., Gattepaille, V., Gros, F., Vourc'h, T., Cornet, J.-F. Radiative Analysis of Luminescence in Photoreactive Systems: Application to Photosensitizers for Solar Fuel Production. *PLoS ONE* 2021, *16* (7), e0255002.

[2] Supplis, C., Gros, F., Dahi, G., Dauchet, J., Roudet, M., Gloaguen, F., Cornet, J.-F. Spectral Radiative Analysis of Bio-Inspired H_2 Production in a Benchmark Photoreactor: A First Investigation Using Spatial Photonic Balance. *International Journal of Hydrogen Energy* 2018, *43* (17), 8221–8231.

[3] Dahi, G., Eskandari, A., Dauchet, J., Gros, F., Roudet, M., Cornet, J.-F. A Novel Experimental Bench Dedicated to the Accurate Radiative Analysis of Photoreactors: The Case Study of CdS Catalyzed Hydrogen Production from Sacrificial Donors. *Chemical Engineering and Processing: Process Intensification* 2015, *98*, 174–186.

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About the author: Fabrice GROS is full professor at Sigma Clermont, France, since 2018. He is engineer in Chemical Engineering of the Grenoble INP, France, where he also obtained a PhD Thesis in Electrochemical Process Engineering in 2005. He obtained in 2017 a HDR at Clermont Auvergne University, France. His current research domains is the study and the modelling of photoreactive processes and their three main applications: photobioreactor, photoreactor, photoelectrochemical cell. He is now the deputy director of studies at SIGMA Clermont Engineering School. He was Head of the Chemical Engineering Department at Sigma Clermont from 2018 till 2021 and Deputy Manager of the "Chemical Engineering, Applied Thermodynamics and Biosystems" axis of the Pascal Institute, France, from 2017 till 2023. He is also president of the scientific association "Committee of Process Engineering Development in Rhône Alpes Auvergne Region", in french "CODEGEPRA, and member of the French National Council of Universities of the 62nd section "Chemical and Thermodynamics Engineering" and of the board of the French Society of Chemical Engineering.

BOOK OF ABSTRACTS

SICHEM – 2024

A – Chemical and biochemical engineering (CBE)

1. Oral presentations

SA-OP01 STUDIES ON ENERGY RECOVERY FROM WASTES USING THE MICROSCALE COMBUSTION CALORIMETER (MCC)

Loredana-Vasilica Postolache[1,*], Ion Anghel[2], Dana Maria Preda[2], Gabriela Șoreanu[1], Igor Cretescu[1] and Gabriela Lisa

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Abstract: *The study of binary mixtures of waste and microalgae residues by microscale combustion calorimetry is presented. The degree of interaction between the mixture components was evaluated by comparing the experimental heat release capacity (HRC) values with those calculated by mass-weighted summation of the HRC values for the pure mixture components. The strongest interaction was found for the binary mixture cardboard* **-** *microalgae residues.*
Key words*: Energy recovery, MCC, Wastes*

Introduction: In view of the current energy crisis, it is necessary to identify potential new energy sources, which is extremely important for the chemical industry, especially for cement plants, which are among the largest energy consumers [1]. In this work, previous studies on energy recovery from waste are continued [2, 3], i.e. the MCC technique [4] is used to measure the heat release properties of microalgae residues (Cho) mixed with waste cardboard (C), textiles (T), plastics (P), tires (A) and used wooden railway sleepers (G).
Experimental: Microscale combustion calorimetry tests were performed under controlled conditions with a temperature rise in the pyrolyser at a heating rate of 1 ºC/s to 750 ºC in nitrogen atmosphere at a flow rate of 80 cm^3/min and a constant combustor temperature value of 900 ºC in nitrogen (80%) and oxygen (20%) atmosphere. HRC (heat release capacity), THR (total heat release), and other parameters to evaluate the heat release characteristics were measured experimentally.
Results and discussions: Figure 1a compares the results obtained for HRC for each waste and mixtures in various proportions with Cho, depending on the amount of residue remaining at the end of the test. In each ellipse in the figure the results obtained for each waste tested in mixture with Cho are concentrated and the optimum values are marked with red circles. The criteria for choosing the optimal compositions were: high HRC and low amount of residue. The non-additivity parameter λ was calculated with equation 1 [5] for the binary mixtures evaluated.

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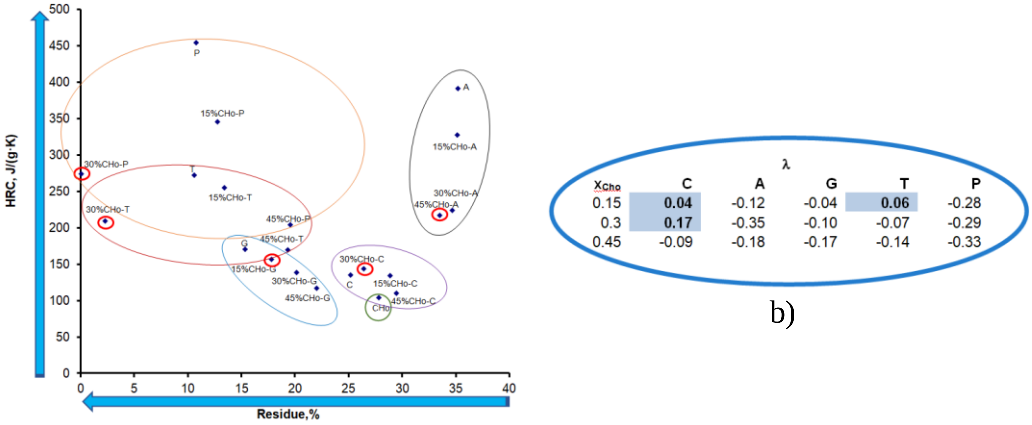
$$\lambda = \frac{\mathbf{HRC_{mixt} - HRC_{add}}}{[\mathbf{x_{Cho}}(\mathbf{1 - x_{Cho}})]^{\mathbf{1/2}} \cdot (\mathbf{HRC_{Cho} + HRC_{waste}})} \qquad (1)$$

where HRC_{mixt} is the experimental value for binary mixtures, HRC_{add} the value calculated according to the HRC additivity law for the individual components in the binary mixture, x_{Cho} the mass fraction of microalgae residues, HRC_{Cho} the experimentally determined value for microalgae residues and HRC_{waste} the experimentally determined value for C, T, P, A and G.



a)

x_{Cho}	C	A	G	T	P
			λ		
0.15	**0.04**	-0.12	-0.04	**0.06**	-0.28
0.3	**0.17**	-0.35	-0.10	-0.07	-0.29
0.45	-0.09	-0.18	-0.17	-0.14	-0.33

b)

Fig. 1 a) Heat release capacity values as a function of percent residue,
b) non-additivity parameter λ

Conclusions: The study found that the use of microalgae residues mixed with different types of waste can increase the energy potential of alternative fuels.

References:

[1] Marenco-Porto C. A., Fierro J.J., Nieto-Londoño C., Lopera L., Escudero-Atehortua A., Giraldo M., Jouhara H., Potential savings in the cement industry using waste heat recovery technologies, *Energy*, 279, (2023), 127810.

[2] Bejenari V., Marcu A., Ipate A-M, Rusu D., Tudorachi N., Anghel I., Sofran I-E., Lisa G., Physicochemical characterization and energy recovery of spent coffee grounds, *J. Mater. Res. Technol.*, 15, (2021), 4437-4451.

[3] Marcu A., Lisa G., Sofran I-E., Anghel I., Serban M., Evaluation of the thermal behaviour of agricultural wastes for possible use in the biomass pellets industry, *Chem. J. Mold.*, 15, 1, 2020, 58-66.

[4] Xu Q., Mensah R. A., Jin C., Jiang L., A critical review of the methods and applications of microscale combustion calorimetry for material fammability assessment, *J.Therm. Anal. Calorim.*, 147, (2022), 6001–6013.

[5] Snegirev A.Yu., Koraiem Handawy M., Stepanov V.V., Talalov V.A., Pyrolysis and combustion of polymer mixtures: Exploring additivity of the heat release rate, *Polym. Degrad. Stab.*, 161, (2019), 245-259.

SA-OP02 TECHNOLOGICAL SOLUTIONS FOR OBTAINING BACTERIAL CELLULOSE MEMBRANES WITH LARGE SURFACE AREA

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Abstract: *A short review examines the possible technologies to have BC membranes with a large surface area. The chosen solution for BC with a large surface area is that of biosynthesis in a rotary drum contactor, for which constructive and operating data are presented.*

Key words: bacterial cellulose, rotary drum reactor, process factors, mathematical modeling

Introduction: Bacterial cellulose (BC) is the purest form of cellulose known to date with special features compared to classic cellulose [1, 2]. Biosynthesis of BC by the action of *Acetobacterium Xilinium (AC)* systems on suitable culture medium [3, 4] can lead to the formation of BC membranes with a large surface area using static, rotating disks, rotating drum and aerated bioreactors [5, 6].

Experimental and modeling: The independent process factors were determined to be the initial pH of the culture medium, total sugars and total microelements in culture medium, drum rotating velocity and aeration quality, while the BC productivity and the state of oxygen concentration in the culture medium were considered the dependent process factors. Figure 1 show the experimental set up, in which the drum reactor is the basic component. A second-order 4-factors experimental design was considered to determine the effect of factors on BC productivity and the state of oxygen concentration in the culture medium.

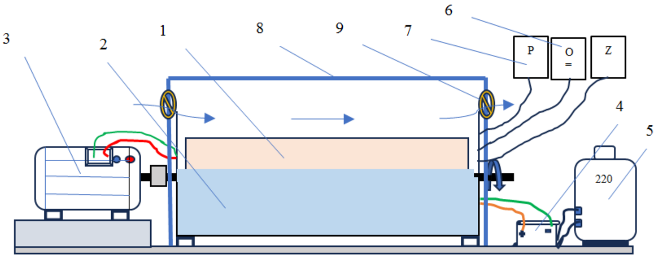

Fig. 1 Laboratory pilot set up for BC synthesis with a drum reactor: 1- drum in reactor; 2- tank for culture medium; 3- drum actuation electric motor; 4- direct current source; 5- current controller, 6 - oxygen meter, 7- pH meter, 8- protection enclosure against culture infection, 9 - air fans

Results and discussions: The results regarding the dependence of BC productivity on the process in the experimental investigation were developed according to 4 factors following a second-order orthogonal plan (SOOP).

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$$x_j = \frac{z_j - z_{jc}}{\Delta z_j} \tag{1}$$

$$x_{jp} = x_j^2 - \frac{\sum_{i=1}^{N} x_{ji}^2}{N} \tag{2}$$

The result, expressed by the response surface $y(x_1,x_2,x_3,x_4)$, leads to Equation (3) regarding the dependence of productivity in raw BC (y) on the 4 process factors (pH, total sugar content, total microelement content, rotation drum velocity) in dimensionless expression. The values of the process factors that maximize the BC productivity of the drum bioreactor were evaluated by solving Equation (4) with solution of Equation (5).

$$y(x_1,x_2,x_3,x_4) = 65.42 + 6.55x_1 + 7.89x_3 - 5.94x_4 + 14.44x_2x_4 - 9.17x_3x_4 + 9.66x_1x_2x_4 + 5.762x_1x_2x_3x_4 - 7.45(x_1^2 - 0.8) - 3.5558(x_3^2 - 0.8) \tag{3}$$

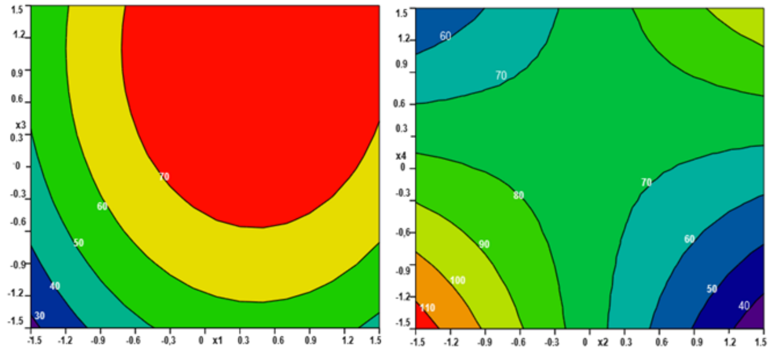

Fig. 2 Contour plot for drum reactor BC productivity versus process factors: $y(x_1,0,x_3,0)$ *vs.* x_1, x_3 (left); $y(0,x_2,0,x_4)$ *vs.* x_2,x_4 (right).

$$\frac{\partial y(x_1,x_2 2,x_3,x_4)}{\partial x_1} = \frac{\partial y(x_1,x_2 2,x_3,x_4)}{\partial x_2} = \frac{\partial y(x_1,x_2 2,x_3,x_4)}{\partial x_3} = \frac{\partial y(x_1,x_2 2,x_3,x_4)}{\partial x_4} = 0 \tag{4}$$

$$x_{1op} = 0.44, x_{2op} = 0.9, x_{3op} = 1.1, x_4 = 001, y(x_{1op}, x_{2op}, x_{3op}, x_{4op}) = 80.5 \tag{5}$$

The factors for the BC productivity of 80.5 kg/m^3 were expressed by pH= 5.5, the sugar concentration in the culture medium of 59 g/L=1, the total microelements content of culture media of ~25 mg/L and the drum rotation speed of 2 rot/min.

Conclusions

The rotary drum bioreactor was selected to produce BC membranes with large surface area. The SOOP plan was used during the experimental investigation, so that the BC productivity of the reactor was expressed analytically. The response surface was analyzed to identify the values of the process factors that ensure the maximization of the BC productivity of the bioreactor.

References:

[1] Dudman W., Cellulose Production by *Acetobacter acetigenum* and other *Acetobacter spp.*, *J . Gen. Microbiol.*, 21, (1959), 312-326.

[2] Hsieh Y.C., Yano H., Nogi M., Eichhorn, S., An estimation of the Young‘s modulus of bacterial cellulose Filaments, *Cellulose*, 15, (2008), 507–513.

SA-OP03 THERMAL TREATMENT AN GREEN TECHNOLOGY IN MEDICALWASTE MANAGEMENT

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Abstract: *Considering the priority of Environmental Protection and Security in the European Union, which is a significant factor for ensuring human health, it is essential to implement and promote various actions aimed at reducing environmental pollution, such as effective waste management strategies.*

In specialist literature and European legislation, hazardous medical waste classification and standard waste classification codes have been given particular importance. The goal of efficient waste management is to minimize the presence of hazardous substances in products and/or substitute hazardous substances with safer alternatives. Due to the potentially detrimental nature of medical waste, there is a need to promote advanced technologies for transforming hazardous medical waste into biogas (methane and carbon dioxide), synthesis gas (hydrogen and carbon monoxide), liquid biofuels (methanol and biodiesel), or pure hydrogen. Additionally, treated hazardous medical waste can be utilized as raw material for co-incineration processes.

The objective of this study is to introduce this thermal treatment technology for hazardous medical waste as a comprehensive business model, effectively integrating all material flows within a circular process aimed at ensuring efficient resource utilization. Consequently, the minimization of thermally treated hazardous medical waste generation is achieved, aligning with the "Best Available Techniques BAT" standards, ultimately contributing to enhancing environmental safety and security.

Keywords: Medical waste treatment facilities, incineration, sterilization, circular economy, pollution, alternative methods, competitive advantage.

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SA-OP04 CONTRIBUTIONS ON THE USE OF VIRTUAL TRAINING IN IMPROVING THE RESPONSE TO CIVIL PROTECTION CONTEXTS

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Abstract: *When some types of hazards manifest themselves severely and trigger large-scale impact disasters, they typically result not only in damage to life, buildings and infrastructure, but also in damage to economic activity, with the potential for cascading effects. This is commonly acknowledged and no demonstration is required. Just as it is no mystery that these effects generate losses for households, businesses, governments, whole society, and the damage needs to be repaired, homes and infrastructure rebuilt and activities resumed.*

Proper preparedness of the response teams ensures higher protection of communities and wider. Recent worldwide events, in particular the SARS COV 19 pandemic, have forced the identification of solutions to enable further training and preparedness activities using innovative methodologies. One example is the use of virtual reality to continue training in such challenging situations.

These pioneering training solutions should enable civil protection stakeholders to be better prepared for natural and man-made disasters and to react faster to limit and mitigate their effects, including in scenarios impacting several countries simultaneously, such as a pandemic.

The present research analysed the results of some exercises (both field and virtual) conducted in the midst of a pandemic wave, based on findings of what worked (for whom, why, under what circumstances) and what needs to be strengthened, in order to build a sound picture of disaster preparedness.

The exercise organised in a virtual context revealed the merits of training using advanced tools but also some limitations compared to field exercises, which would entail the full participation of the response capabilities and not just some components of them.

It can be considered that virtual training can be, with a few caveats, the solution for medium and long term preparedness, even for the purposes of civil protection.

Key words: emergency situations, civil protection, virtual training

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SA-OP05 MODELING AND OPTIMIZATION OF A PROPYLENE GLYCOL PRODUCTION PLANT

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Abstract: *In this work, a conceptual design of a glycerol hydrogenolysis plant to manufacture propanediol was carried out, considering a production capacity of 30000 t/yr. Mass and heat balances, sizing of the main equipment and the economic evaluation was performed using Aspen Plus v10 commercial simulator. The behavior of the tri-phase hydrogenolysis reactor was analyzed both at the level of catalyst pellet and at the catalyst bed. The economic evaluation showed the feasibility of the proposed process flowsheet.*

Key words: Glycerol valorization, conceptual design, process modeling, economic evaluation

Introduction: Glycerol is a valuable raw material, both in terms of the significant quantity obtained as a by-product from transesterification and saponification processes in the biodiesel and soap industries, and due to its potential for chemical and biotechnological transformation into value added chemicals with applications in numerous fields.

Modelling: This work describes the conceptual design of a plant with a production capacity of 30000 metric tons per year of propylene glycol. The mass and thermal balances were carried out using Aspen Plus v10 process simulator.

Results and discussions: The hydrogenolysis reaction occurs in two stages: glycerol dehydration to acetol (hydroxyacetone) followed by acetol hydrogenation to propylene glycol. To achieve industrially relevant glycerol conversion and selectivity towards propylene glycol, a classical $Cu/ZnO/Al_2O_3$ catalyst and a 5:1 hydrogen to glycerol molar ratio were used. The chemical transformation takes place in a three-phase reactor with the solid catalyst in a fixed bed. Using the kinetic model proposed by Zhou *et al.* [1] and mass transfer relations proposed by Korsten and Hoffmann [2], the design of the reactor was carried out considering the influence of the physical mass transport steps at the catalyst pellet scale on overall behavior of the process.

Conclusions: Based on the economic evaluation carried out using Aspen Plus v10 process simulator, the initial investment cost and the annual operating cost were estimated. An estimated propylene glycol cost (1.52 $/kg) lower than the market price (1.96 $/kg) for the year 2023, demonstrates the economic feasibility of the proposed process flowsheet.

References:

[1] Z. Zhou, X. Li, T. Zeng, W. Hong, Z. Cheng, W. Yuan, Kinetics of Hydrogenolysis of Glycerol to Propylene Glycol over $Cu-ZnO-Al_2O_3$ Catalysts, Chinese Journal of Chemical Engineering 18(3) (2010) 384-390.

[2] H. Korsten, U. Hoffmann, Three-Phase Reactor Model for Hydrotreating in Pilot Trickle-Bed Reactors, AIChE Journal 42(5) (1996) 1350 - 1360.

SA-OP06 1,4-BUTANEDIOL SYNTHESIS FROM MALEIC ANHYDRIDE – PROCESS ANALYSIS

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Abstract: *In this work, a conceptual design of a plant for manufacturing 1,4-butanediol from maleic anhydride was carried out, with a production capacity of 50,000 tons per year. Mass and heat balances were performed using the Aspen Plus v10 simulator, and the main equipment characteristics were determined and used to estimate the production price for 1,4-butanediol. Comparing the predicted production price of 2 EUR/kg with the market price 5 EUR/kg, the proposed flowsheet is deemed economically feasible.*

Key words: 1,4-butanediol, maleic anhydride, gas-solid reactor, extractive distillation.

Introduction:

1,4-Butanediol is an important raw material in the synthesis of various polymers, such as polyurethanes and polybutylene terephthalate (PBT) [1].

Modelling: The proposed process flowsheet was evaluated using Aspen Plus v10 commercial simulator, the mass and heat balances were carried out and the characteristics of the main equipment were determined. The MATLAB programming environment was employed for the design and analysis of a gas-solid reactor used for synthesizing 1,4-butanediol from γ-butyrolactone; the process behaviour was evaluated both at the scale of the catalyst pellet and that of the catalyst bed.

Results and discussions: The main characteristics of the gas-solid γ-butyrolactone hydrogenation reactor were determined, resulting in a 25 % conversion and a 20 % 1,4-butanediol yield at the reactor outlet. The effectiveness factor evaluated at the catalyst particle scale (with values between 0.4 and 0.6) showed an important influence of the internal diffusion on the process kinetics.

Conclusions: The importance of the proposed process resides in the purification and marketing of secondary products, while also generating reduced residual streams, aligning with Green Chemistry principles [2].

References:

[1] Sampat, B.G., „*1,4-Butanediol: A Techno-Commercial Profile*”, Chemical Weekly, **2011**, pp. 205-211.

[2] https://www.acs.org/greenchemistry/principles/12-principles-of-green-chemistry.html, accessed on 23.06.2023.

SA-OP07 MODELING OF VOLATILE ORGANIC COMPOUNDS FLOW RATE PRODUCED IN PAINTING INSTALLATIONS FROM AUTOMOTIVE INDUSTRY

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Abstract: *Mathematical modeling of the flow rate evolution of volatile organic compounds obtained from tunnel drying of a freshly painted surface*

Key words: Volatile Organic Compounds, Coating in the Automotive Industry, Paints in the Automotive Industry, Mathematical Modelling

Introduction: Painting techniques in the automotive industry have evolved a lot in the last century due to the rapid evolution of technology. If at first the painting is done manually by brushing the surface of the vehicle, polishing and sanding, and its duration was a few weeks, from the desire to reduce the production time of a car, solutions were sought that would offer faster drying and hardening, thus resulting in enamels. However, due to limited raw materials, it gave way to synthetic chemicals [1]. Thus, the application of multiple layers of primer was introduced, which was later replaced by dip coatings, a more automated process, but dangerous due to the solvent emission of solvent-based paints. Then was proposed anodic deposition coatings, based largely on maleinated polybutadiene resins, which were quickly replaced by cathodic ones due to the better corrosion protection of their modified epoxy resin scaffolds and polyurethane-based reactive crosslinkers [1].

Today, most clearcoats in Europe are based on a two-component (2K-) formulation consisting of an acrylic resin with OH functions and a reactive polyurethane crosslinker. The rest of the world still prefers single-component technology based on acrylic resins and melamine crosslinkers [2].Even though the cost of the basecoat/clearcoat paint process was prohibitive for less expensive automobile lines, it was used on more expensive, high-end automobiles. The environment in vehicle painting factories is contaminated by volatile organic compounds released after the application and drying of the paint on the vehicle surface [1]. The specialized literature presents experimental results and states that the following volatile organic compounds are most often released by using car paints: m/p-xylene, toluene, ethylbenzene and o-xylene [3]. Apart from these, other species of volatile organic compounds are also found in much smaller quantities such as: Butylacetate, Methylchloride, Acrylonitrile, 1-Butene, Octane, n-Propylbenzene, m-Ethyltoluene, p-Ethyltoluene, 1,3,5-Trimethylbenzene, o-Ethyltoluene, 1,2,3-Trimethylbenzene, 1,2,4-Trimethylbenzene [4]. However, the

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variety of aromatic species represents 96.9% of paint emissions from car factories [3]. The interest in the present work is to determine the flow rate of organic volatile compounds (VOC) produced by a dyeing installation with continuous operation. A car paint has in its composition a pigment, a binder, a film agent, a filler, additives, a special pigment and as a VOC precursor, a lot of solvent. During the drying phase of the waxed part, the vaporization of the solvent as VOC in the warm circulated air circulated through the drying tunnel causes it to become charged with VOC.

Modelling: The physical model considered is that of a metal piece with a surface *S* thickness δ that is covered with a film of thickness δ_{f0} that enters the tunnel at a constant speed, *w*. Here occurs the piece heating and solvent vaporization from the paint in the air stream, that flows counter currently with the piece movement, so that at the exit from the tunnel there is no more solvent in the paint film. A simultaneous process of mass and heat takes place in the tunnel.

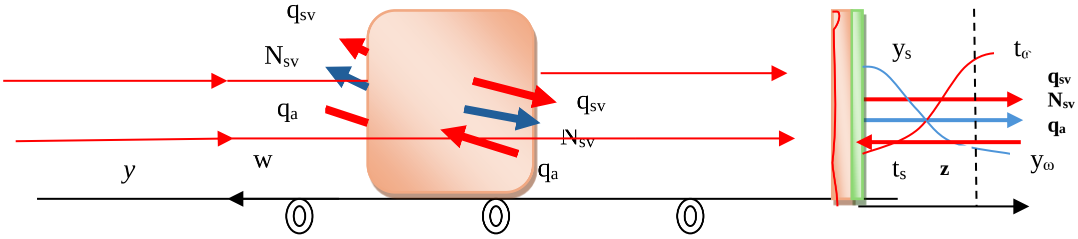

Figure 1. Phenomenology of paint drying in a hot air tunnel

With figure 1 we introduce the description of phenomenology associated with drying of paint deposited on piece of known surface. It insists to shows that here we have simultaneous heat and mass transfer. The right part of figure gives the temperature and COV concentration profiles near to paint surface when the piece is in current position *x* in the tunnel. A mathematical model of tunnel paint drying describes how the solvent concentration (molar fraction) in the paint decreases along the tunnel, respectively how this concentration increases in the drying air.

In order to establish the model equation that shows how the piece temperature evolves along the drying tunnel, it is assumed that it has a high thermal conductivity, so that the heat received is quickly spread throughout its mass. To complete the model, it is also necessary to determine how the air temperature and VOC concentrations change along the tunnel. If H is the drying piece characteristic length, then when it moves from *y* to *y+dy*, it takes heat and discharges solvent vapors. So the drying paint model for a mobile piece in a tunnel where hot air is in a countercurrent contains the differential equations and respectively together with consistent expressions N_{sv}, q_a, q_{sv} and initial conditions that show the state of model differential equations variables at one of the ends of the tunnel. These conditions are written here for hot air entering in tunnel. Here air does not contain VOCs, the piece is almost dry, and it have a temperature close to that of hot air.

The case in which the numerical integration is done from the piece entrance into tunnel has the main condition that here the paint of piece has the solvent molar fraction corresponding to paint application layer. Also, here the entrance piece temperature is that of the paint application environment. This is the case that was used in the simulations performed to prove the model functioning and its ability to analyze the investigated process.

References:

[1] H.-J. Streitberger, K.-F. Dossel, *Automotive Paints and Coatings - Introduction*, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2008, ISBN: 978-3-527-30971-9

[2] Nelson K. Akafuah, Sadegh Poozesh, Ahmad Salaimeh, Gabriela Patrick, Kevin Lawler and Kozo Saito, *Evolution of the Automotive Body Coating Process*, MDPI, 2016, 10.3390/coatings6020024

[3] Bin Yuan, Min Shao, Sihua Lu, Bin Wang, *Source profiles of volatile organic compounds associated with solvent use in Beijing, China*, Atmospheric Environment, Beijing, 2010, 10.1016/j.atmosenv.2010.02.014

[4] M.Y. Song, H. Chun, *Species and characteristics of volatile organic compounds emitted from an auto-repair painting workshop*, Scientific Reports, Korea, 2021,

[5] Bird B. R., Stewart E. W., , Lightftoot N. E., , *Transport Phenomena, Chapter 14, Paragraph 14.6*, 442-443, Second Edition, John Wiley & Sons, Inc., 2002

[6] Leca A., Pop M. G., Prisecaru I., Neaga C., Zidaru Gh., Musatescu, V., Isbasoiu E. C., *Calculation guide. Tables, nomograms and thermotechnical formulas*, vol. II, 71, Technical Publishing House, Bucharest, 1987

[7] Floarea O., Dima R., *Mass Transfer and Specific Equipment, Chapter: Transfer Phenomena Analogy*, Didactic and Pedagogic House, Bucharest, 1984

[8] Welty J., *Fundamentals of momentum heat and mass transfer*, John Wiley & Sons Inc, 2021

[9] Dobre T., Sanchez J. M., *Chemical Engineering Modelling Simulation and Similitude*, Wiley VCH, 2007

[10] Oueslati H., Mabrouk B S., Mami A., *Dynamic Modelling and Performance Optimization-Based Sliding Mode Control of Process Drying in a Convective Tunnel Dryer*, International Journal of System Dynamics Applications, 10, 4, 1-11, 2021

SA-OP08 FUELS FROM WASTE PLASTICS BY PYROLYSIS

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Abstract: *The management of plastic waste has become a pressing global concern due to its environmental impact. In this study, we investigate the conversion of waste plastics into valuable fuels through pyrolysis, focusing on the separation and characterization of the resulting products. The experimental setup involved two types of polymer waste: polyethylene granules (PE) and dirty polyethylene waste. Pyrolysis experiments were conducted on a discontinuous demonstrative unit adapted with a fractionation column. The pyrolysis process was carried out in the absence or presence of zeolite catalysts. Physical and chemical analyses were conducted on the collected fractions. This study underscores the potential of pyrolysis as a viable method for converting waste plastics into valuable fuels. Understanding the composition and properties of the resulting fractions is crucial for optimizing the process and ensuring the quality of the end products.*

Key words: polyethylene, pyrolysis , catalyst, fuels, waste.

Introduction: In the modern era of plastics consumption and production, understanding the chemical processes underlying their synthesis and degradation is essential for sustainable resource and environmental management. A crucial aspect in this area is pyrolysis, a thermal decomposition process that can transform polymers such as polyethylene into simpler substances with diverse applications [1].

Experimental and/or Modelling: *Experimental Setup:* A prototype laboratory setup useded for the conversion of waste plastics into valuable fuels through pyrolysis; *Polymer Waste:* polyethylene (PE). The waste materials were sourced in the form of granules or film.

Results and discussions: The pyrolysis experiments conducted on polyethylene (PE) waste yielded distinct separation efficiencies for each polymer type. For PE, the separation efficiencies were: gaseous fraction (38.3%), naphtha (10.8%), diesel (15.9%), heavy paraffinic fraction (16.6%), and pyrolysis residue (18.3%). Characterization of the fractions indicated the presence of both saturated and unsaturated hydrocarbons, with iodine value analysis confirming the presence of unsaturated compounds. Also, each fraction was analyzed and characterized by total number of carbons that is shown in figure 1. This results have the potential for further processing to enhance the quality of the end products.

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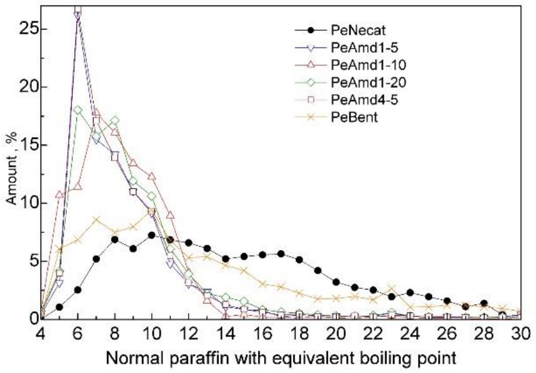

Fig. 1 Total number of carbons using different catalysts on polyethylene

Conclusions: The experimental setup and procedures outlined above allowed for the efficient conversion of waste plastics into valuable fuels through pyrolysis, providing valuable insights into the separation and characterization of the resulting products.

References:

1. Evode, N., et al., *Plastic waste and its management strategies for environmental sustainability.* Case Studies in Chemical and Environmental Engineering, 2021. **4**: p. 100142.

SA-OP09 EFFECT OF AXIAL MIXING IN MODELLING OF THREE PHASES STEADY STATE GASOLINE HYDROFINING

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Abstract: *The reducing as much as possible of the size of a three-phase model of gasoline hydro-refining obliges to accept a co-current plug flow structure for gas and liquid. The real flow of gas phase and liquid over the fixed bed expressing the catalyst can be considered accepting that each fluid phase flow is affected by axial dispersion. The stationary model thus developed contains a system of five second order differential equations coupled with mass transfer equations for* H_2 *and* H_2S *and the S compound whose concentrations on catalyst surface are controlled by chemical reaction.*

Key words: gasoline hydrofining, three-phase model, hydrofining catalysis, species mass transfer

Introduction: In gasoline hydrofining with a proper catalyst and hydrogen excess, compounds with nitrogen are hydrogenated faster than those with sulfur. Considering that on the catalyst the hydrogenation rates of alkyl sulfides and alkyl disulfides of aromatic sulfide compounds are the same, the hydrofining can be reduced then to a simplified process where we remove the sulfur compounds as a single one [1, 2].

Mathematical modeling: In three phases model of hydrofining the catalyst (solid phase) is covered by liquid (liquid phase) which is surrounded by the gas phase, which can be considered as the continuous phase [3]. Chemical reaction take place only at the solid catalyst, where S is converted by H_2 to H_2S. A balance for H_2, H_2S and S respect to a small control volume with dimension *Sdz*, at *z* position in column, can be build. To obtain the surface reaction concentration of reactive species (H_2, H_2S, S) the steady state of process imposes the equality of surface reaction rate with liquid phase species transport rate toward surface (Eq. (1) – (3))

$$\boldsymbol{\rho_{vc} v_R (C_{Ss}, C_{H2s}, T) = K_{lH2} \sigma_{sl} (C_{H2l} - C_{H2s})} \tag{1}$$

$$\boldsymbol{\rho_{vc} v_R (C_{Ss}, C_{H2s}, T) = 0.5 K_{lH2S} \sigma_{sl} (C_{H2Ss} - C_{H2Sl})} \tag{2}$$

$$\boldsymbol{\rho_{vc} v_R \big(\rho_{vc} v_R (C_{Ss}, C_{H2s}) = k_{lS} \sigma_{sl} (C_{Sl} - C_{Ss})\big) = k_{lS} \sigma_{sl} (C_{Sl} - C_{Ss})} \tag{3}$$

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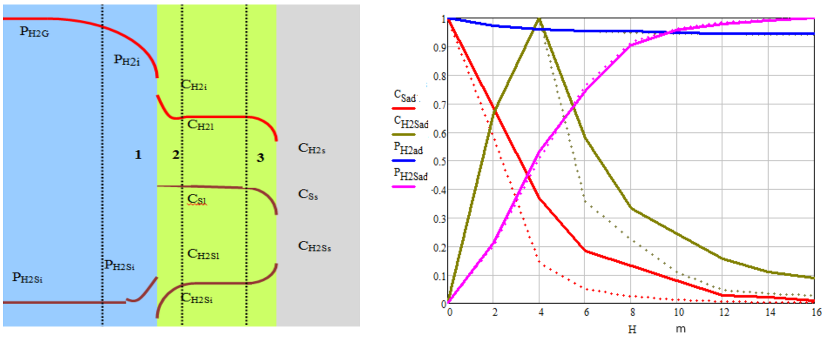
For *Shell DC-2532 Co-Mo* base catalyst, for mild severity operation at low to moderate operating pressure, the reaction rate, in kmol$_r$/kg$_c$s, is given [4] below:

$$\boldsymbol{v_R(\rho_{vc}v_R(C_{Ss},C_{H2s})} = \frac{4.27\ 10^9 \exp\left(\frac{131990}{RT}\right) C_{Ss} C_{H2s}^{0.45}}{\left(1+41770\ exp\left(\frac{2761}{RT}\right) C_{H2S\ s}\right)^2} \tag{4}$$

Simulation results: Figure 2 concentrates the results of one case model integration for given process parameters, while the model computed dimensionless species concentration along of catalytic bed considering *H* height.



(a) **(b)**

Fig. 1. Hydrofining simulation: (a) concentration profiles for H_2 and H_2S; (b) evolution of dimensionless process responses for an imposed height of catalyst bed (T = 650 K, p = 55 bar, $w_l = 2\cdot10^{-5}$ m/s, $w_g=4\cdot10^{-4}$ m/s, dashed lines: without axial mixing)

Respect to data from figure 2(b) we note that: i) the effect of axial mixing in the gaseous phase is weak, the curves for the partial pressure of H_2 and for the partial pressure of H_2S overlap those specific to the case $D_G = 0$; ii) the effect of axial mixing in the liquid phase gives at the exit from the column (H = 16 m) a concentration of S and of H_2S over the specific one of the process simulation without considering the axial mixing; iii) S is removed from gasoline from 0.038 mol/L to 0.00009 mol/L, without axial mixing, respectively 0.00012 mol/L; iv) the intensity of the process is very high in the first 6 m of the reactor.

Conclusions: We have shown that liquid axial mixing is important for advanced gasoline sulfur removal, and despite the fact that the process takes place very intensively in the first few meters of the reactor, high catalyst bed is required.

References:

[1] Jimenez F., Nunez M., Kafarov V., *Study and modeling of simultaneous hydrodesulfurization, hydrodenitrogenation and hydrodearomatization on vacuum oil hydrotreatment*, European Symposium on Computer Aided Processes, Editors Pujganer I., Espuna A., Elsevier Science, 2005

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

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

SA-OP010 PURIFICATION OF SODIUM LIGNOSULFONATE BY PARTIAL PRECIPITATION AND CROSS-FLOW FILTRATION ON CERAMIC MEMBRANES

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Key words: sodium lignosulfonate, ceramic membranes, cross-flow microfiltration

Introduction: Sodium Lignosulfonate (NaLS) is a very useful by-product of the sulfite pulping process that has the purpose of eliminating lignin from a wood source to produce a cellulose rich raw material for the paper and cardboard industry. An effective way of purifying NaLS with the goal of further valorization is to use ultrafiltration [1]. However, the effectiveness and feasibility in this case is strongly dependent on the mean molecular weight of the sodium lignosulfonate. To circumvent this problem a partial precipitation method is used to facilitate the partial aggregation of sodium lignosulfonate chains.

Experimental: NaLS obtained from CCH (Drobeta-Turnu Severin) was processed using an XLab 5 cross-flow filtration system by passing it through a 5 μm membrane, recovering the permeate which was subsequently passed through a 500 nm ceramic membrane. Following this, the permeate was spray dried. The NaLS powder was used to make solutions of varying concentrations which were precipitated with varying solvents. The volumes used to precipitate were also different. The precipitates were analyzed by TEM/EDX.

Results and discussions: The morphological of the precipitates and compositional information showed a new possibility to achieve an intensified purification although it was shown large enough particles are obtained only if the initial stream is concentrated enough. The optimal point depends on overall costs. The highest recovery yield is not necessary economical. With this new information, several cross-flow filtration experiments were performed at both high shear and low-shear conditions. The results suggest that the centrifugal pump might not be compatible with this approach for larger industrial application.

Conclusions: The cross-flow filtration / partial precipitation coupled approach was investigated to obtain sufficient purification of Sodium Lignosulfonate. It was

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shown that even with a low mean molecular weight some separation/purification is still achievable. This method should yield much better results with a ligher mean molecular weight.

References:

[1] Nath, Kaushik, Vinay B. Patel, Haresh K. Dave, and Suresh C. Panchani. "Valorisation of sodium lignosulfonate by ultrafiltration of spent sulphite liquor using commercial polyethersulfone membrane." Indian Chemical Engineer 64, no. 5 (2022): 553-564.

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SA-OP011 ESTIMATING THE PURITY OF SODIUM LIGNOSULFONATE IN BROWN LIQUOR USING TEM/EDX

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Key words: sodium lignosulfonate, transmission electron microscopy, cross-flow microfiltration

Introduction: Sodium lignosulfonate (LSNa) has been obtained for a long time as a by-product of the paper and cardboard industry in the sulfite pulping process. It is produced in very high quantities (400 kt worldwide per year in 2022 [1]) as a derivative of lignin which is found in large quantities in trees. It can be valorized as a surfactant, plasticizer, binder, dispersant for concrete and others [2]. A key factor to maximize its properties with respect to possible applications is its purity, especially in relation to its salt content. TEM/EDX can offer a wealth of information and it will be applied this way in the current work.

Experimental: LSNa recovered from CCH (Turnu-Severin) was prefiltered using vacuum filtration to remove large debris or other insoluble material. Afterwards, it was fed to the Pall Membralox XLab 5 cross-flow filtration system fitted with a Membralox ceramic membrane with a pore size of 5 μm. The permeate was recovered and fed to the same system fitted this time with a 500 nm Membralox ceramic membrane. The permeate was spray dried. LSNa/glycerol films were produced by drying at 60 °C. The required necessary concentration was estimated to produce films ~50 nm on the TEM grid for TEM-EDX characterization. Plasma cleaning and sample volume where varied. Carbon film copper grids (Ted Pella, Inc.) were used. XRD analysis of the powders was used to determine the composition in terms of sodium sulfite, sodium sulfate and sodium lignosulfonate.

Results and discussions: The dried permeates (at 5 μm and 500 nm) were used to determine the minimum glycerol content for achieving stable films. After drying, the thickness of the films was measured which allowed the estimation of the film density. This allowed to estimate the volume and concentration necessary to achieve a 50 nm film by drying.

Conclusions: This method can be used to estimate purity and to recover other information concerning the purity of any sodium lignosulfonate stream.

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References:

[1] ChemAnalyst - Sodium Lignosulphonate Market Analysis: https://www.chemanalyst.com/industry-report/sodium-lignosulphonate-market-731, accesed 25th of March 2024

[2] Aro, T. and Fatehi, P., 2017. Production and application of lignosulfonates and sulfonated lignin. ChemSusChem, 10(9), pp.1861-1877.

Acknowledgment: This work was supported by Ministry of Research, Innovation, and Digitization, CCCDI—UEFISCDI, project number PN-III-P2-2.1-PTE-2021-0675, within PNCDI III, 74PTE ⁄ 2022.

SA-OP012 PYSICAL – CHEMISTRY ASPECTS OF METHYLENE BLUE AND ITS ANALOGUE'S ADSORPTION FROM AQUEOUS ENVIRONMETS

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Abstract: *Methylene Blue (MB) is one of the most often used organic dyes. In medicine, besides its employment as a disinfectant, it is also widely used in biological staining, for marking various cells and tissues. Whatever its utilization, its discharge is a significant source of pollution to any water body. Adsorption is a suitable low cost and highly effective mean of undesired dye removal from various wastewaters [1]. It has been carried on solid adsorbents of diverse sources, from the usual sawdust to the fly ash - industrial [2], and the raw mango seed - agricultural [3] wastes, respectively. This work deals with the comparative investigation of some kinetic and thermodynamic aspects of methylene blue and one of its recently synthetized [4] analogue's adsorption onto standardized filter paper, from synthetic aqueous solutions. The employed MB analogue was 3,7-bis(bis(2-hydroxyethyl)amino)phenothiazine-5-ium iodide (MBI), a water soluble, hence more likely pollutant species. All experiments were carried out in triplicate glass batch arrangements. In the case of methylene blue, the advance of the process with total solid-liquid contact time was monitored photometrically at 664 nm. Five kinetic [1, 5] and eight thermodynamic [1, 6] models were tested against experimental data. It has been found that at constant temperature and adsorbate/adsorbent ratio, the kinetic profile of the overall process will be closer to a pseudo-second order model at low MB loads, whereas with its increasing concentration, the intra-particle diffusion will gain importance. Experimental data proved that the glass vessel itself adsorbed significant dye amounts, yet this decreased with initial MB loads. The adsorption isotherm of MB at 298K is likely to be described by a Freundlich equation. The temperature dependence of the process kinetic parameters suggest a mixed physical and chemical sorption. Similar measurements were carried out for MBI and the data are compared and discussed.*

Key words: Methylene Blue, Adsorption kinetics, Adsorption thermodynamics

References:

[1] Yagub M.T., Sen T.K., Afroze S. 1, Ang H.M., Dye and its removal from aqueous solution by adsorption, *Adv. Colloid Interface Sci.*, 209, (2014), 172-184.

[2] Kumar K.V., Ramamurthi V., Sivanesan S., Modeling the mechanism involved during the sorption of methylene blue onto fly ash, *J. Colloid Interface Sci.*, 284, (2005), 14-21.

[3] Kumar S.P, Palaniyappan M., Priyadharshini M., Vignesh A.M., Thanjiappan A., Fernando P.S.A, Ahmed R.T., Srinath R., *Environ Prog Sust Energ*, 33, 1, (2013), 87-98.

[4] Gál M, Turza A., Stoean B, Găină L, Cristea C, Gál E., Lovász T., Porumb D., Silaghi-Dumitrescu L., Alternative procedures for the green synthesis of 3,7-bis(N,N-(2-hydroxyethyl)amino)phenothiazinium dye, *Studia UBB Chemia*, 67, 4, (2022), 303-314.

[5] Csavdari A., Detailed kinetics of diffusion driven adsorption processes, *Studia UBB Chemia*, 68, 3, (2023), 179-189.

[6] Bitay E., Csavdari A., Some unmodifies household adsorbents for the adsorption of benzalkonium chloride – A kinetic and thermodynamic case study for commercially available paper, *Toxics*, 11, 12, (2023), 950.

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https://www.chem.ubbcluj.ro/

SA-OP13 MASS TRANSFER OF H_2 IN AQUEOUS MEDIA FOR BIOLOGICAL METHANATION: INFLUENCE OF MICROORGANISMS AND OPERATING CONDITIONS

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Abstract: *The hydrogen gas-liquid mass transfer rate was investigated in a jacketed stirred cell using different media under various operating conditions. The mass transfer limitation was quantified and demonstrated.*

Key words: Biological Methanation, Hydrogen, CO_2 Reuse, Gas-Liquid Mass Transfer.

Introduction: Biological methanation can convert hydrogen gas to methane by hydrogenating CO_2 in the liquid medium using anaerobic microorganisms [1]. In this process, the main kinetic limitation of the reaction rate is the low solubility of H_2 in aqueous media, which induces a low rate of gas-liquid mass transfer. Thus, the volumetric mass transfer coefficient (k_La) was measured [2].

Experimental and Modelling: The experimental apparatus consists of a jacketed stainless steel cell with magnetic stirrer equipped with a microsensor capable of recording the H_2 concentration in the liquid phase over time. The k_La was determined for different operating parameters: temperature (25/45°C), gas flow rate (50-200 $mL.min^{-1}$), gauge pressure (0-3 bar). The aqueous medium includes deionized water (reference), or Basal Anaerobic (BA) medium without/with enriched mixed *Archae* cultures (volume: 500 mL) [3]. Gas was dispersed using a micro-sparger with controlled porosity. The assumption of perfect mixing was used for k_La estimation.

Results and discussions: In Figure 1, the experimental results show an increase in k_La of H_2 as a function of temperature and gas flow rate. However, a general decrease was observed when the pressure increased. Under atmospheric pressure, k_La was higher in the BA medium due to the effect of salts on the gas-liquid interfacial area. This trend, however, was reversed at higher pressure.

The results on bubble size show that H_2 bubbles were usually higher than air bubbles under similar conditions and that the mean bubble size increased with pressure, which can explain the k_La decrease with high pressure.

In Figure 2, the results show that the biological medium slightly increased k_La, while the effects of pressure and H_2 gas flow rate remained the same. The detailed results with microorganisms are not shown in the chart because the tests are still ongoing, but H_2 content was decreased and could approach zero due to hydrogen

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consumption by the methanogens despite the high excess in H_2 in the gas phase (4:1 CO_2 to H_2 ratio) and the high gas flow rate.

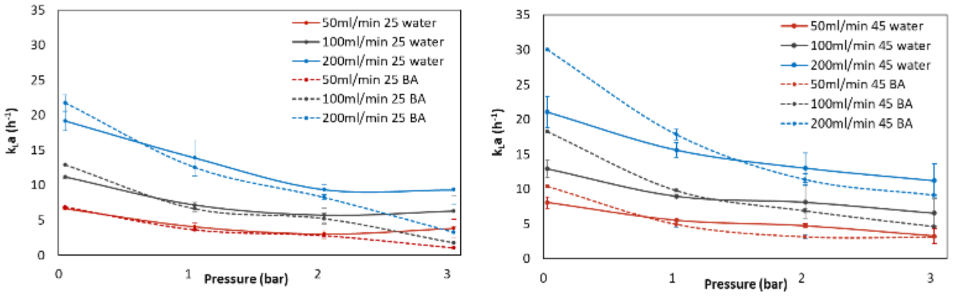

Fig. 1 k_La of H_2 in deionized water and BA medium without microorganisms with different temperature, gas flow rate and gauge pressure.

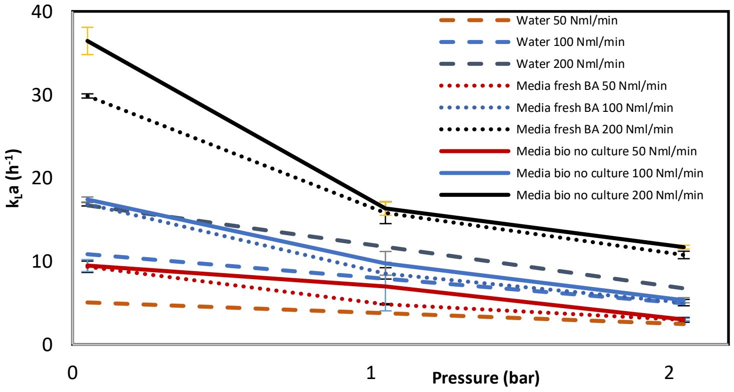

Fig. 2 k_La of H_2 in deionized water, fresh BA medium, and biological medium after centrifuge without microorganisms in 45°C for different gas flow rate and gauge pressure.

Conclusions: The limitation of H_2 mass transfer to liquid media in biological methanation was highlighted and quantified in the presence of methanogens even at high H_2 gas flow rate. The type of gas phase, H_2 and air, influenced the bubble size. k_La decreased when pressure increased due to the increase in bubble size with pressure, which highlights the key role of the sparger on bubble size and mass transfer rate.

References:

[1] Lecker B., Illi L., Lemmer A., Oechsner H., Biological hydrogen methanation – A review. Bioresource Technology, 2017, 245 (2017), 1220-1228.

[2] Rusmanis D., O'Shea R., Wall D. M., Murphy J. D., Biological hydrogen methanation systems – an overview of design and efficiency. Bioengineered, 2019, 10(1), 604-634.

[3] Bu F., Dong N., Khanal S. K., Xie L., Zhou Q., Effects of CO on hydrogenotrophic methanogenesis under thermophilic and extreme-thermophilic conditions: Microbial community and biomethanation pathways. Bioresource Technology, 2018, 266 (2018), 364-373.

SA-OP14 EFFECT OF TEMPERATURE AND EMULSIFIER DOSAGE ON WATER SEPARATION FROM CRUDE OIL EMULSION

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Abstract: *Crude oil emulsions are formed during the extraction process, especially due to the violent mixing of crude oil with water. Emulsions formed in this way can create problems in refineries, such as corrosion of processing or transport equipment.*

Demulsification is a method of separating emulsions from water in crude oil into the constituent phases and which can be achieved by mechanical, thermal, electrical or chemical methods (using demulsifiers). Thermal and chemical demulsification methods are often use together for a better efficiency of water separation from crude oil emulsion because the demulsifier under the increasing temperature, accelerates the emulsion breaking process. Demulsifiers displace the natural stabilizers present in the interfacial film around the dispersed water droplets in the emulsion.

In this work, three different crude oil emulsion were prepared with different brine concentration in crude oil as follow: 10%, 15% and 20% (v/v). From these three emulsions, only the 10% sample was selected for the experiment due to its high stability. Also, the separation time and the percent of water decanted from different crude oil emulsions was determined at different temperatures (30, 40, 50 and 60ºC) and for different concentrations of demulsifier in emulsion (1%, 2%, 3%, 4% and 5%). The demulsifier selected for this work is a commercial type used in industrial applications, consists from a mixture of C_9 *aromatics hydrocarbons. Bottle test method was used to measure the water separation from crude oil emulsions. Also a Bresser 5201000 LCD Digital Microscope, with 40x magnification level, was used to observe the water droplets distribution in crude oil emulsion. The results show that the efficiency of water separation from water-in-oil emulsions increases with increasing temperature and demulsifier concentration. Consequently, for a faster demulsification rate, a higher temperature is recommended, but not exceeding 60°C, as above this value there is a risk of losing the lighter fractions of crude oil through vaporization.*

Key words: Crude oil, demulsification, emulsion, demulsifier, bottle test.

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SA-OP15 LABORATORY LEACHING TESTS AS METHOD TO EVALUATE THE SOIL HEALTH

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Abstract: *Laboratory tests aimed at assessing the leaching of free species from the soil can provide information on its pollution state. In order tom estimate the effect of rain on soil leaching soil samples were washed repeatedly and in the effluent was determined the inorganic carbon, total carbon, total nitrogen and eluable metal ions.*

Key words: Soil leaching, Soil pollution, Inorganic carbon, Total carbon, Free nitrogen, Ion exchange, Eluable ions

Introduction: Soil with various active (fertilizer, microelements, macroelements, organic and inorganic pollutants and others) compounds, present or added, can be analyzed respect to its health or respect to it comportment to rainfall by and column leaching [1]. Different water flow rates in leaching simulate high rainfall and low rainfall environments. Objectives of our paper respect to nutrient mobility were: (i) develop a technique to demonstrate non binded compounds movement in the soil, (ii) establish a set of procedures and equipment to obtain leached species concentration from column selected samples (iii) determine nutrient mobility.

Experimental and/or Modelling: A simple experimental device where the soil fixed bed is irrigated with distilled water and the washing product is collected as samples at time intervals was used. The water flowrate is ensured by dripping, controlled with the help of a perfuse system. Each sample is analyzed to determine the compounds estimated to be chemically unbound in the complex soil structure. Each sample is analyzed to determine the compounds estimated to be chemically unbound in the complex structure of the soil. From the point of view of mathematical modelling the leaching of one species from fixed soil bed occurs upon dispersion flow model coupled with a interphase soil-water species transfer that is associated with a lent soil swelling. With c_{vs} and c_{ss} the one transferable species concentration in water respectively in solid, at position x and time τ, the announced mathematical model [2-4] is expressed by assembly of relations (1)- (4). Along with the basic equations of the model (1), (2), we recognize that the model requires the knowledge of the specific interphase equilibrium of the transferable species (k_d in the relation (3)) and considers that the soil swelling in the rigid physical lbed occurs with the reduction of the soil pores size (4).

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$$\frac{\partial c_{vs}}{\partial \tau} + \frac{w_l}{\epsilon}\frac{\partial c_{vs}}{\partial x} = D_l\frac{\partial^2 c_{vs}}{\partial x^2} + k_l\sigma(c_{vs}^*(c_{ss}) - c_{vs}) \qquad (1)$$

$$\frac{\partial c_{ss}}{\partial \tau} = -k_l\sigma(c_{cs}^*(c_{ss}) - c_{vs}) \qquad (2)$$

$$c_{vs}^*(c_{ss}) = k_{ds}c_{vs} \qquad (3)$$

$$\varepsilon = \varepsilon_0\exp(-a\tau) \qquad (4)$$

$$x = 0,\quad \frac{w_l}{\epsilon}c_{vs\,in} = -D_L\frac{dc_{vs}}{d\tau} \qquad (5)$$

$$x = H,\quad \frac{dc_{vs}}{dx} = 0 \qquad (6)$$

The relations (5) and (6) give the initial integration conditions for a system where flow occurs with axial dispersion. The model can use leaching dynamics data in order to identify its characteristic parameters. However, some independent measurements are also needed, for example to identify the parameters from the expression of the liquid fraction in the layer

Results and discussions: As I have shown, one of the aims of the work was to highlight the evolution of the leaching intensity of some species from the soil depending on the intensity and duration of some rains. Table 1 shows the conditions of intensity and duration of the rain considered in the experimental investigation using a soil sample taken from UPB park from Polizu location.

Table 1. Rain intensity and duration for soil leaching experiments.

Sample	u.m	P1	P2	P3	P4	P5	P6	P7	P8
Rain Intensity	l/(m^{2}h)	30	20	10	30	30	20	20	10
Duration	h	1	1	0.5	1	0.5	1	0.5	1
Relax time	h	0	0	0	14				

Figure 1 shows the state of inorganic and total carbon leached after each of those 8 leching case. We observe here the relatively fast regeneration, after 14 hours in the present case, of the inorganic carbon. This suggests that it is either the consequence of the dissociation of some carbonates with a fairly high solubility product or more.

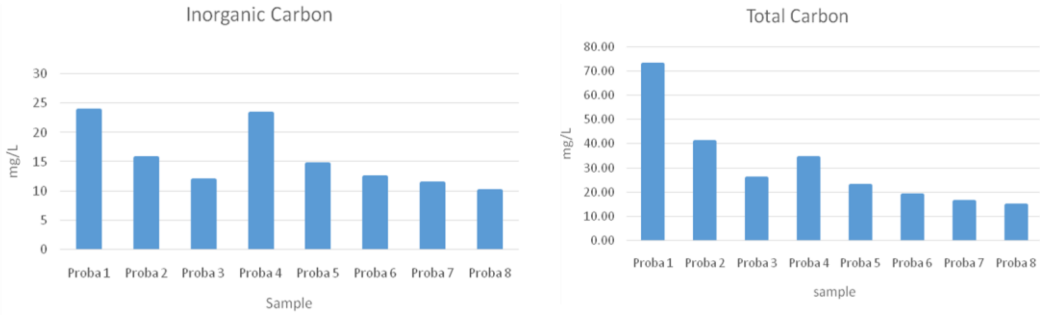

Fig. 1 Concentration of inorganic and total carbon at soil leaching upon rain intensity and duration.

Figure 2, which shows the dynamics of organic carbon and free nitrogen concentration (urea, ammonium nitrate, amines. etc.) in the leaching water at bed exiting shows, as interesting, that: i)) the leachable nitrogen is still washed away after the first rain and does not appear anymore after the relaxation between the rains, which clearly indicate that in the soil nitrogen compounds are extremely weakly linked to the soil components, ii) organic carbon is much better bound to the soil structure components so that it is more difficult to release from the soil.

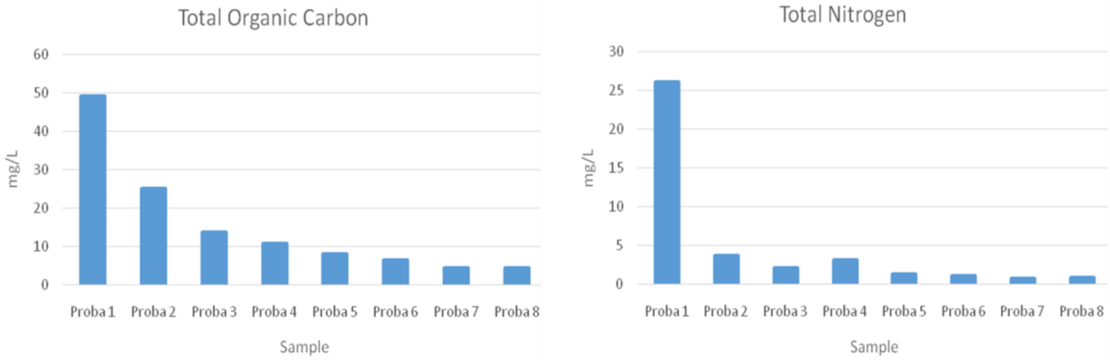

Fig. 2 Concentration of organic carbon and of free nitrogen at soil leaching upon rain intensity and rain duration.

We have shown that a bed of 10 cm of soil is depleted in leachable compounds quite quickly when the intensity and duration of the rain are considerable. It is understood, however, that the leachable compounds will be found active in the soil at depths of more than 10 cm. For some plant species this is good, for others the impoverishment of the superficial soil start is undesirable, it must be corrected. Without going into details, we show that the leaching of the three species, above presented, indicates that the case soil sample indicates t a healthy (unpolluted) soil.

Conclusions: The paper provides data on characterization of leaching from the soil of chemically unbound species upon rain intensity and duration. The leaching problem of these species can also be characterized by modeling, such a model being presented here.

References:

[1] Bowman R.S., Auer C.G., Jaynes B.D., *Water flow and chemical retardation in soils: A simple effective laboratory demonstration*, J. Agron. Educ., 17, 38 -40, 1988

[2] Dobre T., Sanchez J, M., *Chemical Engineering Modelling, Simulation and Similitude*, Wiley VCH, 2007

[3] Owens S.D., Johnson G. V., *Fertilizer Nutrient Leaching and Nutrient Mobility: A Simple Laboratory Exercise*, J. Nat. Resources Life Sci. Educ., 25, 2, 128-133, 1996

[4] Revil A., *Transport of water and ions in partially water-saturated porous media. Part 1. Constitutive equations*, Advances in Water Resources 103, 119–138, 2017

SA-OP16 STOCHASTIC MODELING OF THE PROCESS OF TERTIARY EXPLOITATION OF CRUDE DEPOSITS

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Abstract: *In the petroleum industry, given the complex nature of the processes and phenomena involved, uncertainties are significant. Until recently, efforts to integrate uncertainties have been limited, with the industry predominantly focused on deterministic approaches. It is now clear that in order to make effective investment and development plans we must understand the uncertainties related to the deposit and integrate them into the analysis until the end goal. The present material brings into play the phenomenological understanding of the Tertiary movement of crude oil in abandoned fields.*

Key words: *Oil, tertiary flow enhanced*

Introduction: Uncertainty is the inability to accurately estimate a value. Risk is the probability of a negative outcome, relative to a predefined objective. By construction, the single models paradigm can never be used to quantify the uncertainties of a prediction. In addition, it gives the false illusion that we are able to predict behavior that is actually complex, non-linear and uncertain. In the oil and gas industry, abandoned fields are sometimes modeled for reopening, but tertiary migration of hydrocarbons is rarely considered.

This is precisely why it is necessary to create a numerical model that provides optimization data:

a. liquid flow rate, crude oil flow rate, water flow rate on the total deposit and on groups of wells.

b. The amount of liquid in the deposit,

c. The amount of crude oil in the field.

Experimental and/or Modelling: Based on the developed algorithm (an analysis of the Differential Evolution of the deposit) we minimized the amount of water associated with the crude oil and maximized the amount of crude oil. Thus we obtained the new, optimized assembly (crude oil flow). To exemplify the tertiary migration process, three scenarios will be analyzed comparatively. Time is one of the most important factors in the tertiary migration process. Previous studies and observations from field tests have confirmed that for noticeable results the period of rest must be of the order of decades.

The first scenario assumes the continuation of exploitation after the end of the production history in exactly the same regime. The second involves the shutdown of all wells for a period of 10 years and the third shutdown for a period

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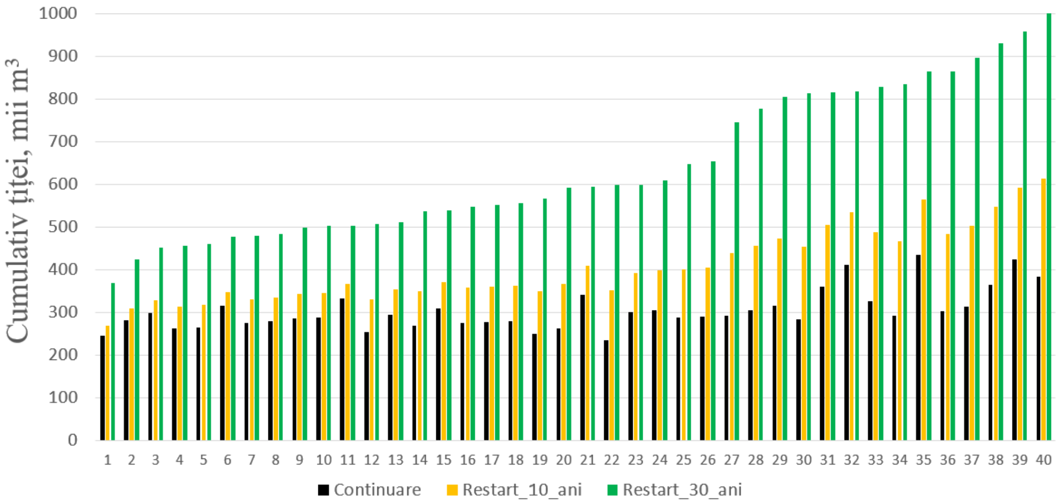
of 30 years. Based on these scenarios, the pressure and saturation data will be compared in the first case right at the moment when the production history ends, for the second case, before the resumption of exploitation after 10 years of activity, and for the third case before the resumption of the activity after 30 years of inactivity. The cumulative totals of crude oil obtained over a fixed period of 10 years for each case will also be compared.



Conclusions: The case study carried out shows that the tertiary migration process makes the crude oil reserve after a period of 30 years from the abandonment to be approximately 300 thousand m^3 higher than the one evaluated when the exploitation stopped

References:

[1] I. Duțu, D. Stoianovici, T. Chiș, D. Bârsan, D. Sulaiman - Transition Zone Analysis in Oil Reservoirs with Mixed or Preferential Water Wettability, JENRR.98480, 2023

SA-OP17 EFFECT OF CORROSIVE ENVIRONMENT ON OFFSHORE DRILLING PLATFORMS

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Abstract: *In the Romanian territorial waters of the Black Sea there are several fixed installations built before 1989 or in the immediately following years, installations that followed the Romanian standards of the time and less the international ones from the design phase. Moreover, they currently show a greater or lesser degree of degradation due to environmental factors that have acted on them over time or due to ineffective maintenance. This is why, in this paper, we will refer quite frequently to these installations with the presentation of their condition, but also of the measures that must be imposed to extend their life.*

Key words: *Oil and gas, Offshore platforms, corrosion*

Introduction: Offshore structures, both fixed and mobile, are metal or metal-reinforced concrete constructions, intended to support oil and gas exploration and/or production installations under conditions of extreme external demands such as: loads as a result of gravity (the own weight of the installations), loads developed by environmental factors (wind, waves, sea currents, marine vegetation), seismic loads or even accidents. Thus, the components of offshore structures can be subjected to permanent stresses of various intensities (horizontal or vertical movements, vibrations) which can give rise to mechanical stress. Also, the corrosion of the components plays a very important role in the process of degradation of the installations. On the seas and oceans of the world there is an impressive number of offshore structures designed in such a way as to comply with the provisions and international standards in force. The type of request, the structural analysis of each type of installation, as well as the required checks are discussed within these standards. The design of an offshore installation is analyzed so that it meets all the requirements and robustly copes with both normal exploitation and extreme conditions. During operation, significant design changes lead to a reassessment of structural integrity that must be done in accordance with the updated design project. In this case, new structural resistance calculations will be made to ensure that the requirements of the regulations are met.

Experimental and/or Modelling: The marine atmosphere contains chlorides in the presence of very high humidity. The breaking of waves (especially at the shore) leads to the formation of fine droplets in the atmosphere that evaporate, thus resulting in chlorides that are then scattered by wind and sea currents. Thus, Chlorine ions (Cl^-) appear on the surface of the metals and break through the

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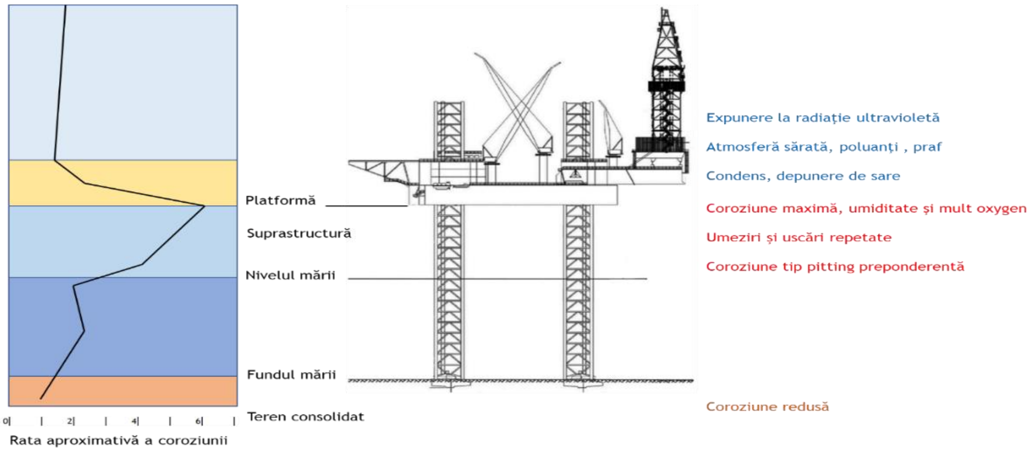
protective layer. The corrosion rate decreases significantly once we move offshore, being even 10 times lower at 300 meters from the shore compared to the area in its immediate vicinity. For ordinary steel the corrosion rate is 0.125 mm/year (25 mg/dm^{2}day). Constructions partially immersed in seawater can also be corroded due to differential aeration. The part close to the surface, which will be constantly bathed by waves, will always have a film rich in O_2 on the surface, which will constitute the cathodic zone where the reduction of oxygen will take place, and the metallic part from the depth, where access to O_2 is difficult, will constitutes the anodic zone on which the dissolution of the metal will take place.



Conclusions: The series of international standards applicable to types of offshore structures (ISO) constitute a common basis covering those aspects that address the design requirements and evaluations of all offshore structures used by the oil and natural gas industry worldwide. By applying them, the intention is to achieve adequate levels of reliability for manned and unmanned offshore structures, regardless of the type of structure and the nature or combination of materials used.

References:

[1] Corrosion risk assessment and safety management for offshore processing facilities, OFFSHORE TECHNOLOGY REPORT 1999/064, https://www.hse.gov.uk/research/otopdf/1999/oto99064.pdf

BOOK OF ABSTRACTS

SICHEM – 2024

A – Chemical and biochemical engineering (CBE)

2. Poster presentations

SA-P01 STATISTICAL ANALYSIS OF URBAN AIR QUALITY IN PLOIESTI, ROMANIA DURING AUTUMN

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Abstract: *This research focused on the impact of air pollutant emissions and weather conditions on urban air quality in Ploiesti, Romania. We statistically analyzed the data collected by air quality monitoring stations, focusing on PM_{10}, SO_2, NO_2, CO pollutants, and meteorological parameters from 01.09.2023-30.11.2023 in Ploiesti, Romania. The data were processed according to the limits allowed by the environmental legislation in Romania. We investigated the correlations between weather parameters and pollutant concentrations, followed by a detailed statistical analysis. Ploiesti Municipality hosts 2 stations for monitoring emissions from traffic, 2 background stations and 2 stations for monitoring industrial emissions. Results and discussions reveal the daily concentrations of pollutants, presented in the form of box plots diagrams. These graphs illustrate the minimum variation, lower and upper quartile, median and extreme values, with their concentration in November. For example, we observed the largest decrease in average nitrogen dioxide (NO_2) concentration in September for one monitoring station (PH-6) compared to the other two stations. These fluctuations are influenced by factors such as road traffic density, weather conditions, vehicle types and industrial emissions. The study highlights the critical importance of addressing air pollution due to road transport in metropolitan areas in Romania. It is imperative to adopt effective policies and measures to reduce the impact of air pollution on public health and the environment.*

Key words: air, urban, statistics

Introduction: Air pollutant emissions and weather conditions contribute to urban air quality [1]. In this study, we statistically investigated data collected on urban air pollution using air quality monitoring station measurements. Long-term monitored pollutants were PM_{10}, SO_2, NO_2, CO and meteorological parameters from 01.09.2023-30.11.2023 in Ploiesti, Romania.

Experimental and/or Modelling: Data were processed according to the limit value allowed under the Romanian environmental legislation. Correlations were made between weather parameters and pollutant concentrates. They were then statistically analyzed. Ploiesti municipality includes 2 stations for monitoring emissions from traffic, 2 background stations and 2 stations for monitoring industrial emissions.

Results and discussions: Figure 1 shows daily concentrations of pollutants over time as box plots diagrams. The graphical representation illustrates the minimum value, the lower quartile, the upper median quartile and the maximum value.

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Extreme values are predominantly found in November. For nitrogen dioxide (NO_2), the average concentration decrease in September for the PH-6 station is the highest compared to the other two monitoring stations (55.01%). In the analysis of the concentration of particulate matter for PH-5 with an aerodynamic diameter of 10 micrometers (PM_{10}) we find a slight decrease for October compared to September, after that followed an upward trend for November, with a percentage increase of 37.59%. These fluctuations are due to the density of road traffic, meteorological parameters, vehicle types and industrial emissions.

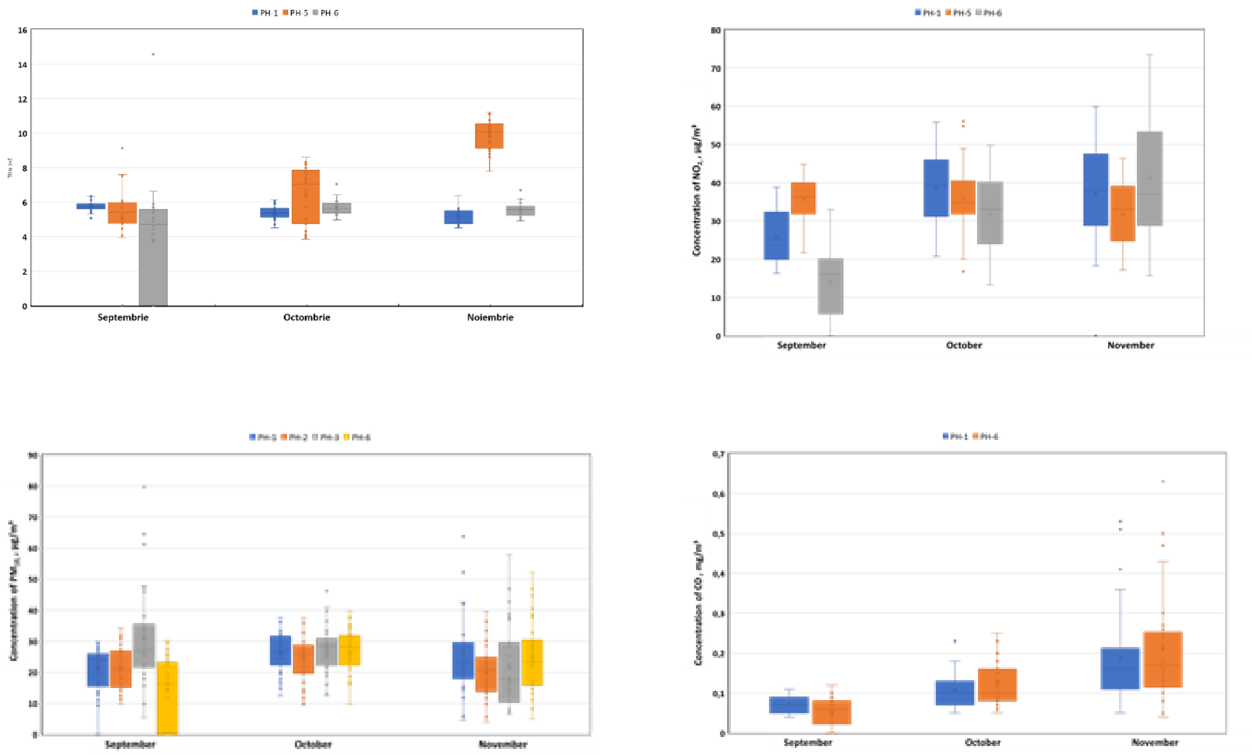

Fig. 1 Statistical summary of the level of air pollution in the form of box plants in September, October, November of CO, NO_2, SO_2 and PM_{10}

Conclusions: The study highlights the crucial importance of addressing air pollution due to road transport in metropolitan areas in Romania.

References:

[1] Güzel, T.D. and Alp, K., The effects of technological developments in transportation vehicles on air pollution mitigation of metropolitan cities: A case study of Istanbul, *Sci. Total Environ.*, 912, 2024.

SA-P02 APPLICATION OF (BIO)CHEMICAL ENGINEERING CONCEPTS AND TOOLS TO MODEL GENETIC REGULATORY CIRCUITS (GRCs), AND SOME ESSENTIAL CCM PATHWAYS IN LIVING CELLS FOR THE *IN-SILICO* RE-DESIGN SOME GRCs TO OBTAIN GMOs

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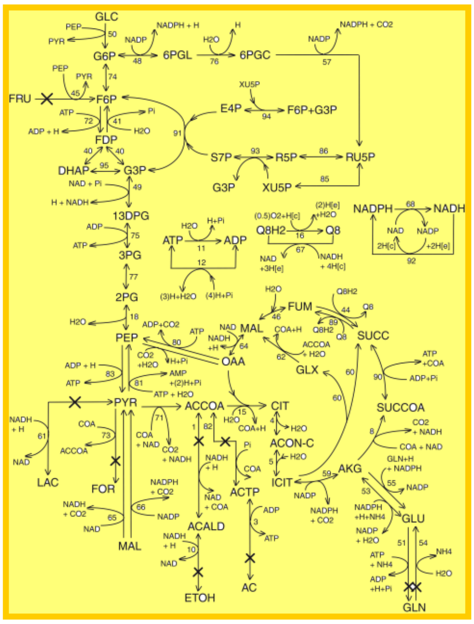
Abstract:



The *E.coli* **CCM** structured reduced model of Maria et al., 2011 [6].

*The paper is aiming at reviewing the main math modelling and computational tools developed by Maria [rw5-rw8] to in-silico re-design genetic regulation circuits (**GRC**) in living cells to get genetically modified micro-organisms (**GMOs**) of desired characteristics. A number of suggestive case studies are reviewed as well. More specifically, this work is aiming to prove the feasibility and the advantages of using the novel concept to couple extended cell-scale **CCM**-based (central carbon metabolism) structured deterministic kinetic models with bioreactor classical dynamic models (including macro-scale state variables). The ever-increasing availability of experimental (qualitative and quantitative) information, at the cell metabolism level, but also on the bioreactors' operation necessitates the advancement of a systematic methodology to organise and utilise these data. The resulted hybrid structured modular dynamic (kinetic) models (**HSMDM**), promoted by the author, were proved to successfully solving more accurately difficult bioengineering problems. In such **HSMDM**, the cell-scale model part (including nano-level state variables) is linked to the biological reactor macro-scale state variables for improving the both model prediction quality and its validity range. In all case studies, there are multiple advantages of using extended **HSMDM**-s. for the in-silico designed genetically modified (**GMOs**). In other words, this work presents a holistic "closed loop" approach that facilitate the control of the "in vitro" through the "in silico" development of **HSMDM** with continuous variables, and based on cellular metabolic reaction mechanisms.*

- *case study no.1 (hg). **HSMDM** is used to simulate the dynamics and to optimize the mercury uptake from wastewaters in a semi-continuous (**SCR**) three-phase fluidized bioreactor (**TPFB**). Thus, a higher prediction detailing degree is reported, that is prediction of the dynamics of [26(cell species) + 3(bulk species)] vs. only [3 (bulk species)] by a classical macroscopic **SCR- TPFB***

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*model, while covering a wider range of input mercury loads, with using cloned E. coli cells with various amounts of mer-plasmids [**Gmer**]. Also, the model allows predicting the bacteria metabolism adaptation to environmental changes over dozens of cell cycles, and the optimum [**Gmer**] level leading to an optimum mercury uptake without exhausting the cell resources.*

- *case study no.2 (trp). **HSMDM** is used to simulate the dynamics of a fed-batch bioreactor (**FBR)** at both cell- and bulk-phase species levels, aiming to maximize the tryptophan (**TRP**) production. The **HSMDM** realizes a higher prediction detailing degree, by predicting the dynamics of [11(cell species) + 4(bulk species)] vs. only [3 (bulk species)] by a classical macro-level **FBR** model, while covering a wider range of control variables, and various **GMO** E. coli cells strains. Eventually this model was used to derive the optimal operating policy of a **FBR** leading to the **TRP** production maximization, by considering a larger number of control variables related to the bioreactor feeding.*
- *case study no.3 (succ). **HSMDM** is used to simultaneously maximize two opposite objectives, that is the production of biomass and of succinate (SUCC) in a batch bioreactor (**BR**). By using the **HSMDM** a Pareto-optimal front was generated including the locus of the all best compromise problem solutions, that is the cell **CCM** optimal fluxes, together with the genes to be in-silico removed from the genome ("gene knockout") to design E. coli mutants that simultaneously fulfil the two goals. This approach uses a mixed-integer nonlinear programming (**MINLP**) rule, coupled with an effective adaptive random search to determine the optimal **CCM** metabolic fluxes of the **GMO** in respect to the two goals, and associated to the "gene knockout" strategies. The **MINLP** alternative using the **HSMDM** model is proved to be superior to the linear procedure **MILP** (mixed-integer linear programming) that solves a combinatorial problem in a bi-level optimization approach, of dimensionality sharply increasing with the number of removed genes, rapidly becoming not applicable. Besides, in this case study, the **HSMDM** realizes a higher prediction detailing degree, by predicting the metabolic fluxes dynamics of [72(cell species), involved in 95 reactions + 1(bulk species, i.e. the biomass)] vs. only [1 (bulk species)] by a classical macroscopic **BR** model, while covering a wider range of control variables, and GMO E. coli strains.*

Key words: systems biology; cell metabolism; deterministic modelling; gene expression modelling; genetic regulatory circuits (GRC); Pareto design of *E.coli* to obtain maximum succinate; design cloned *E.coli* to get maximum mercury uptake; design *E.coli* with a genetic switch biosensor; design *E.coli* with a desired glycolytic oscillator; tryptophan synthesis; glycolytic oscillator; Phenyl-alanine synthesis in *E. coli*; kinetic models for the central carbon metabolism (CCM); "whole-cell of variable-volume" (**WCVV**) modelling framework; "hybrid structured modular dynamic (kinetic) models" (**HSMDM**); "modular structured dynamic (kinetic) models" (**MSDKM**)

References:

[rw-5]. Maria, G., 2023, Application of (bio)chemical engineering concepts and tools to model GRCs, and some essential CCM pathways in living cells. Part 1. Generalities, Curr Trends in Biomedical Eng & Biosci., (Juniper publ, Irvine CA, USA), 22(1), 556080-556104 (2024). DOI: 10.19080/CTBEB.2023.22.556080

[rw-6]. Maria, G., 2024, Part 2. Mathematical modelling framework, Annals of Reviews & Research, (Juniper publ, Irvine CA, USA), 10(3), pp. 555790-555835, doi: 10.19080/arr.2024.10.555790

[rw-7]. Maria, G., 2024, Part 3. Applications in the bioengineering area, Archives in Biomedical Engineering & Biotechnology, (Iris publ, San Francisco CA, USA), 7(5), (2024), abeb ms.id.000672. doi: 10.33552/abeb.2024.07.000672.

[RW-8]. Maria, g., 2024, part 4. Applications in design some GMO-s, annals of systems biology, (Ppeertechz Publ, Los Angeles, USA), 7(1), 001-034, 2024, article id: asb-7-121, https://doi.org/10.17352/asb.000021

SA-P03 STOCHASTIC MODELING OF COPPER CEMENTATION IN SYSTEM WITH LIQUID FLOW BY INTENSE PERCOLATION

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Abstract: The paper analyses the stochastic modelling of copper cementation on iron in a system with perfect mixing of contacting phases as in the case of contact by percolation with a high liquid flow rate when the solid (iron balls, iron particles) is in a fixed or fluidized bed. The phenomenological model with stochastic two states regarding the surface process (Cu is deposited as a result of surface reaction, which can be fast, respectively Cu leaves as micro particles from the surface) contains as model parameters the volume mass transfer coefficient (k_{la}), the kinetic constant of surface copper deposition frequency (α), the kinetic constant of surface copper removal frequency (β). The interest of the paper is to show how these parameters depend on process factors.

Key words: cementation process, mass transfer, stochastic modelling, fluidized bed, fixed bed

Introduction: The electrochemistry of the cementation process shows that the presence of Cu and Fe ions in a solution, close to an iron surface, leads to $Cu^{2+}(aq) + 2e^{-} \rightarrow Cu(s)$ with $\varepsilon^{\circ}_{\text{red Cu}} = +0.34$ and $Fe^{2+}(aq) + 2e^{-} \rightarrow Fe(s)$ with standard reduction potential $\varepsilon^{\circ}_{\text{red Fe}} = -0.44$ V [1, 2]. This difference between $\varepsilon^{\circ}_{\text{red Cu}}$ and $\varepsilon^{\circ}_{\text{red Fe}}$ may indicate that the overall surface reaction, $Cu^{2+}(aq) + Fe(s) \rightarrow \rightarrow Fe^{2+}(aq) + Cu(s)$, occurs at high rate [3].

Experimental and mathematical modelling: Basically, cementation occurs through paired electrochemical cells, located on the surface of iron particles. Equation (1) is obtained if the liquid flow fits to perfect mixing structure [3].

$$\frac{c_A}{c_{A0}} = exp\left(-\frac{A_0}{V}k_l\left(\tau\left(1-\frac{\alpha}{\alpha+\beta}\right)+\frac{\alpha}{(\alpha+\beta)^2}\exp(-(\alpha+\beta)\tau)\right)\right) \quad (1)$$

where c_A and c_{A0} are momentary and initial copper ions concentration in liquid phase, A_0 is the iron surface where cementation occurs, V is liquid phase volume, k_l establish the values of copper ions mass transfer coefficient towards solid surface, τ is time whereas α is the kinetic constant of surface copper deposition frequency and respectively β gives the kinetic constant of surface copper removal frequency. It identifies that k_l, α and β are the model factors, which have values established by the independent factors of cementation procedure.

The liquid velocity through fixed bed of iron particles velocity can be over

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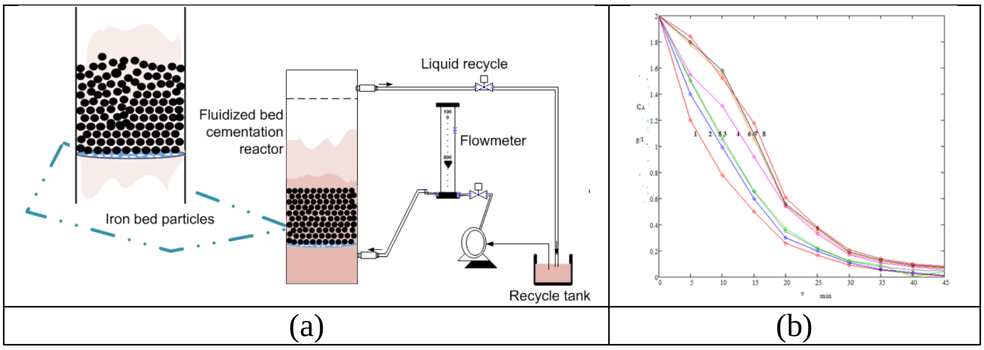

(a) (b)

Fig. 1 Fluidized bed copper-iron cementation device: (a) Experimental set up;
(b) Dynamics of copper ion in liquid for experiments 1-8

fluidization velocity when downward liquid flow is used, as can be observed in Figure 1(a). The initial liquid phase composition (1g/L Cu^{+2} and 0.2 g/L H_2SO_4) and the ratio of liquid mass to initial iron ball mass and bed characteristics (50 kg_l/kg_s, $d_b = 0.001$ m, $h_0 = 0.08$ m, $D_c = 0.04$ m) were set.

Results and discussions: 11 curves of the dynamics of copper ions concentration in liquid, of which the first 8 in which the dimensionless variables x_i i=1, 2, 3 have values between *-1* and *1*, are presented in Figure 1(b).

The response *y* was correlated to the dimensionless factors x_1, x_2 and x_3:

$$\boldsymbol{y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3} \quad (2)$$

Data processing from Equations (3) - (5) shows their dependency upon dimensionless velocity of the liquid through the bed (x_1), upon dimensionless concentration of Cu^{2+} dispersed in the liquid (x_2) and upon dimensionless temperature (x_3).

$$\boldsymbol{k_l = 1.178\,10^{-4} + 1.842\,10^{-4} x_1 + 1.229\,10^{-6} x_2 x_3} \quad (3)$$

$$\boldsymbol{\alpha = 0.012 - 3.67\,10^{-3} x_1 - 3.583\,10^{-3} x_2 x_3 - 3.358\,10^{-4} x_1 x_2 x_3} \quad (4)$$

$$\boldsymbol{\beta = 0.068 - 0.012\,x_1 - 0.014 x_2 x_3 - 0.015 x_1 x_2 x_3} \quad (5)$$

Conclusions: A cementation model with stochastic components particularized to fixed bed cementation with high liquid flow rate percolation was developed for perfect mixing phases contact. The experimental investigation considering the flow rate through the bed, the content of powdered *Cu* in liquid and the working temperature as process factors allowed the identification of model parameters dependence on these process factors.

References:

[1] Nadkarni, R. M., Wadsworth, M. E. Kinetic study of the cementation of copper with iron, *Advances in Exraction Metallurgy*, IIM., London, 1976, 919-941.

[2] Nadkarni R. M., Jelden C. E., Bowles K. C., Flanders H. E., Wadsworth M. E., A kinetic study of copper precipitation on iron, *Trans. Met. Soc.* AIME, 239, 1967, 581.

[3] Duru J. M., Dobre T., Parvulescu O. C., Danciu T., Deleanu I., Raducanu C. E., Stochastic Modelling of Coupled Diffusion and Surface Reaction at Copper Cementation on Iron, Oral

SA-P04 NEURAL NETWORK MODELING OF THERMODYNAMIC EXCESS PROPERTIES

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Abstract: *In this paper, based on the experimentally determined thermodynamic properties (density and refractive index) of 34 binary and ternary mixtures with n,n-dimethylacetamide (x_1), butyl acetate (x_2) and water (x_3), we assessed the excess thermodynamic properties, i.e. excess molar volume. A database containing 136 series of data was thus created and statistically processed with the specialized software SigmaPlot 11.00. The obtained database was used to build neural network models correlating excess molar volume with composition, normalized temperature and refractive index.*

Key words: Excess molar volume modeling; ANN; n,n-dimethylacetamide; butyl acetate; water

Introduction: Chemical plant design requires very accurate data on thermodynamic properties and, in the absence of experimental data, accurate predictive methods are needed. Artificial neural networks (ANNs) have proven capable of solving complex tasks in a number of practical applications. ANN-based models for thermodynamic excess properties provide high accuracy, which is a major advantage in engineering applications [1].

Experimental: Our further research on the determination of the thermodynamic properties of binary and ternary systems [2,3] consisted of experimental determinations of the density and refractive index of the mentioned liquid mixtures at four temperatures: 20, 30, 40 and 50°C, respectively, and at atmospheric pressure. The refractive index of pure liquids and binary and ternary mixtures was determined with an Abbe refractometer with a wavelength corresponding to Na (589.3 nm) and a Lauda E100 thermostat. Density was measured with a DMA 5000 Densimeter.

Results and discussions: The validation stage [4, 5] is the most important stage in any neural model creation process. In this stage, data sets that were not used in the training stage are used and the reliability of the created models is checked. Figures 1a and 1b compare the experimental values with those calculated with the ANN(4:16:1) and ANN(4:12:4:1) models in the validation stage. The obtained correlation coefficients are greater than 0.98, while the standard deviation calculated with equation (1) is 0.063 and 0.061, respectively.

$$\boldsymbol{\sigma} = \sqrt{\sum_{\mathbf{i=1}}^{\mathbf{k}} \left[\mathbf{Vm}_{\mathbf{experimental}}^{\mathbf{exc}} - \mathbf{Vm}_{\mathbf{model}}^{\mathbf{exc}}\right]^{\mathbf{2}} / (\mathbf{n}-\mathbf{p})} \qquad (1)$$

where n is the number of experimental data and p is the number of parameters.

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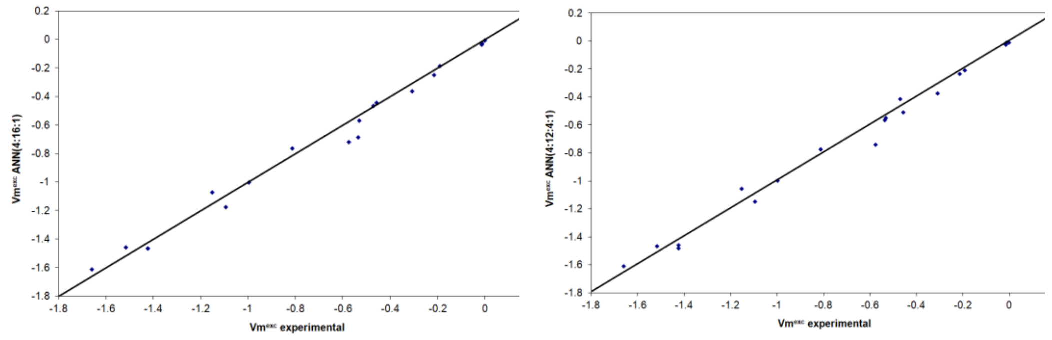

a) b)

Fig. 1 Excess molar volume values calculated with the ANN (4:16:1) (a) and ANN (4:12:4:1) (b) models compared with the experimental values of the validation step

Conclusions: For binary and ternary systems containing n,n-dimethylacetamide, butyl acetate and water, the evaluation of the thermodynamic excess properties based on experimental measurements of density and refractive index, respectively excess molar volume was performed, obtaining the best performance with ANN(4:16:1) and ANN(4:12:4:1) models. The standard deviations for these models in the training stage are 0.023 and 0.022, respectively, and in the validation stage 0.063 and 0.061, respectively.

Acknowledgements: The authors thank the company ROFAROM SRL Miercurea Ciuc, for the support provided for measuring the density with the DMA 5000 equipment.

References:

[1] Karunarathne S.S., Chhantyal K., Øi L.E., ANN-Based Correlations for Excess Properties to Represent Density and Viscosity of Aqueous Monoethanol Amine (MEA) Mixtures, *Proceedings of SIMS EUROSIM 2021Virtual, Finland, 21-23 September 2021*, (2021), 116-122.

[2] Bîrgăuanu I., Danu M., Lisa C., Leon F., Curteanu S., Ibanescu C., Lisa G., Deviation Modeling for Binary and Ternary Mixtures of Benzyl Alcohol-N-Hexanol-Water, *Materials* 15, 16, (2022), 5699.

[3] Bîrgăuanu I., Lisa C., Leon F., Curteanu S., Lisa G., Modeling of excess molar volume for binary and ternary mixtures of benzyl alcohol, n-hexanol and water, *Environ. Eng. Manag. J.*, 22, 12, (2023), 2157-2164.

[4] Barberis A., Aerts H.J.W.L., Buffa F.M. Robustness and reproducibility for AI learning in biomedical sciences: RENOIR, *Sci. Rep.* 14, (2024), 1933.

[5] Hassija V., Chamola V., Mahapatra A., Singal A., Goel D., Huang K., Scardapane S., Spinelli I., Mahmud M., Hussain A., Interpreting black-box models: A review on explainable artificial intelligence, *Cogn. Comput.* 16, (2024), 45–74.

SA-P05 PROCESS OPTIMIZATION FOR BASE METALS RECOVERY FROM WASTE PRINTED CIRCUIT BOARDS USING THE ELECTROCHEMICAL REGENERABLE $KBr/HBr/Br_2$ SYSTEM

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Abstract: *This work presents our results concerning the optimization of the operational parameters involved in the process of base metals recovery from waste printed circuit boards (WPCBs) using the electrochemical regenerable* $KBr/HBr/Br_2$ *system.*

Keywords: waste printed circuit boards, base metals recovery, selective electroextraction

Introduction: Our previous results proven that the electrochemical regenerable $KBr/HBr/Br_2$ system represents a feasible solution for the base metals (BM) recovery from WPCBs [1-5]. Even if leaching solutions based on hazardous pure Br_2 were used, the initial setup led to modest performances as cathodic and anodic current efficiencies of 43.6% and 58.4%, and specific energy consumptions over 0.65 kWh/kg of treated WPCBs and 3.5 kWh/kg of recovered metals [1]. To overcome these drawbacks, leaching solutions without Br_2 and an improved experimental setup were tested.

Experimental: The new experimental setup included mainly a divided electrochemical reactor (ECR), a rotating-drum chemical reactor inserted in the anolyte flow circuit, a pump and a computer-controlled galvanostat. Before each set of experiments, the anodic and cathodic flow circuits were filled with fresh solutions of 2M KBr + 0.5 M HBr. Different amounts of $CuBr_2$ were added in the starting catholytes. The compositions of the resulting electrolytes and deposits were evaluated by flame atomic absorption spectroscopy.

Results and discussions: Using the setup described above, the BM from more than 10 WPCBs samples were successfully leached. Initially, Br_2 is generated in-situ until the first quantities of Cu and Fe were leached. Next, the Cu(II)/Cu(I) and Fe(III)/Fe(II) redox couples become the main leaching agents, stopping the bromine generation. Moreover, the resulting anolytes and catholytes can be replaced reciprocally for pure Cu recovery on cathode and leaching solution regeneration on anode.

Conclusions: We demonstrated that the exposed BM from WPCBs can be successfully recovered using the KBr/HBr system without Br_2 addition. Using this original approach and optimized parameters, improved current efficiencies (over 90%) were obtained. Also, the global specific energy consumption was preserved

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around 0.65 kWh/kg of treated WPCBs and significantly decreased to 2.1 kWh/kg of recovered BM. Noticeably, after the anolyte/catholyte reciprocal switch, high purity Cu deposits (over 99.5%) can be obtained in parallel with the regeneration of the leaching solution.

References:

[1] S.-A. Dorneanu, *Studia UBB Chemia*, 62(3), (2017), 177-186.
[2] S.-A. Dorneanu, E. Covaci, F. Imre-Lucaci, G.L. Turdean, *Studia UBB Chemia*, 64(2), (2019), 555-565.
[3] S. Varvara, S.-A. Dorneanu, A. Okos, L.M. Muresan, R. Bostan, M. Popa, D. Marconi, P. Ilea, *Materials*, 13(16), (2020), 3630.
[4] M.-I. Frîncu, E. Covaci, S.-A. Dorneanu, P. Ilea, *Studia UBB Chemia*, 65(3), (2020), 33-44.
[5] M.-I. Frîncu, E. Covaci, S.-A. Dorneanu, P Ilea, *Studia UBB Chemia*, 66(2), (2021), 137-149.

SA-P06 PHENOL ADSORPTION STUDY ONTO TWO TYPES OF VIRGIN MICROPLASTICS IN FIXED AND FLUIDIZED-BED COLUMNS

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Abstract: *The world pollution level has reached a new stage with the discovery of microplastics and their harmful consequences to the environment. Even though their singular presence represents a major danger, it has also been established that they can behave as transport vectors for certain types of pollutants. Among these various types of chemicals, one of great interest are represented by the group of phenols and its derivatives [1,2,3].*

The first part of the experiment consisted in determining the phenol adsorption capacity of unused polypropylene (PP) and expanded polystyrene (PS) microplastics, both from pure water (solution pH=2) and from sea water (solution pH=7). The polystyrene had a much higher adsorption capacity (8.52 mg/g PS at pH=2 and 52.9 mg/g PS at pH=7, respectively) than the polypropylene (0.46 mg/g PP at pH=2 and 0.249 mg/g PP at pH=7, respectively). Since increasing the pH from 2 to 7 leads to six times increase of the PS adsorption capacity, the same has the opposite effect on the PP adsorption capacity which is halved. The higher adsorption capacity of polystyrene against polypropylene is mainly attributed to the surface properties of the polymers as well as its chemical structures.

The second part of the experiment consisted in dynamic conditions for removal of phenol from water. The column filled with polymer is crossed from bottom to top by an aqueous solution of phenol at a linear velocity of 0.075 cm/s, allowing an efficiency of 39% phenol removal for polystyrene and 15.4% for polypropylene.

References:

[1] H. H. Al Mamari, Phenolic Compounds: Classification, Chemistry, and Updated Techniques of Analysis and Synthesis, Phenolic Compounds, IntechOpen, 2021

[2] L. Fu, J. Li, G. Wang, Y. Luan, W. Dai, Adsorption behavior of organic pollutants on microplastics, Ecotoxicology and Environmental Safety, 217, (2021), 112207, https://doi.org/10.1016/j.ecoenv.2021.112207

[3] A. Tubic, M. Loncarski, S. Maletic , J. Molnar Jazic, M. Watson, J. Trickovic and J. Agbaba, Significance of Chlorinated Phenols Adsorption on Plastics and Bioplastics during Water Treatment, *Water*, 11, 11, (2019), 2358, https://doi.org/10.3390/w11112358

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SA-P07 EXTRACTION OF BIOACTIVE COMPOUNDS FROM WILD GARLIC (*Allium ursinum* L.)

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Abstract: *Wild garlic (Allium ursinum L.) extracts offer a wide range of complex and structurally diverse compounds with antifungal, antibacterial, and antiviral properties. The experimental extraction studies focused on the selection of extraction methods for obtaining primary extracts of wild garlic leaves enriched in chlorophyll pigments (chlorophyll a and chlorophyll b) and carotenoids, with applications in the food, pharmaceutical, and cosmetic industry. The experimental results indicated that Soxhlet extraction was more efficient than ultrasound-assisted and microwave-assisted extraction.*

Key words: Wild garlic, extraction, chlorophyll *a*, chlorophyll *b*, carotenoids

Introduction: Wild garlic contains quercetin, natural pigments (chlorophyll *a* and *b*, carotenoids), vitamins A and C, vitamins from the B complex, mineral salts, and proteins. Wild garlic has a high concentration of bioactive principles, therefore it has benefits for human body (detoxifying, antiseptic, antiviral, and antimicrobial effects) [1].

Experimental: Ultrasound-assisted extraction (80 °C and 40 kHz for 30 min) and microwave-assisted extraction (119 W for 30 min) were used as green methods for primary extraction of leaves pigments (Fig. 1). The conventional extraction method was performed using a Soxhlet extractor (80 °C). Extraction methods complied with ecological principles by using two solvents water and ethanol (1:1 hydroalcoholic mixture).

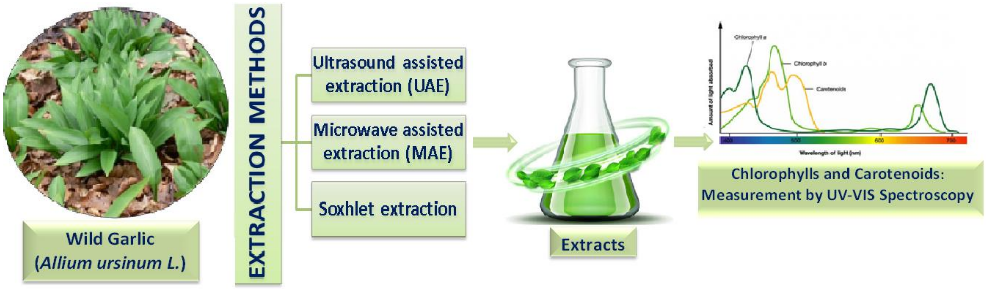

Fig. 1. Extraction of chlorophyll *a*, chlorophyll *b*, and carotenoid pigments from wild garlic.

Results and discussions: Chlorophyll *a*, chlorophyll *b*, and total carotenoid contents were determined using an UV-Vis spectrophotometer at various

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wavelengths (470, 645 and 662 nm) [2]. The results obtained from this analysis highlighted that the classic method (Soxhlet) was the most effective, obtaining contents of chlorophyll and carotenoid pigments of 28.64 µg/mL and 3.95 µg/mL, respectively.

Conclusion: The highest levels of chlorophyll *a*, chlorophyll *b*, and total carotenoid contents were obtained using Soxhlet extraction.

References:

[1] Bernaś E., Słupski J., Gębczyński P., Ražná K., Žiarovská, J., Chemical composition and genome pattern as a means of identifying the origin of preserved wild garlic (*Allium ursinum* L.) in Poland, *Agriculture*, 14(1), 20, (2024). https://doi.org/10.3390/agriculture14010020

[2] Tomsone L., Kruma, Z., Spectrophotometric analysis of pigments in horseradish by using various extraction solvents, (2019), 210-215. https://doi.org/10.22616/FoodBalt.2019.023

SA-P08 METHYLENE BLUE ADSORPTION IN AN AQUASORB L27 ROTATING BED SYSTEM

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Abstract: *This research investigates an intensive discontinuous process for methylene blue dye adsorption from an aqueous solution, in a rotating bed system, containing a specific adsorbent, Aquasorb L27, with enhanced retaining qualities. Experiments were conducted at two different rotational speeds, of 500 and 1000 rpm, and two different temperatures, of 20°C and 45° C, to study the color removal efficiency in this system. A discoloration of approximately 90% is attained at the largest investigated rotational speed, after 40 min at room temperature and after 16 min, at 45°C, respectively. Based on a screening evaluation, the bed spinning speed was found as the most significant influence parameter for the adsorption process.*

Key words: adsorption, rotating bed, intensive process

Introduction: Dye pollutants from various industries, such as textile, paper, and dye manufacturing, pose significant environmental challenges due to their persistence and potential harmful effects on ecosystems. In recent years, there has been growing interest in alternative intensive approaches, for example, use of rotating adsorbent beds, which offer advantages such as enhanced mass transfer rates and potential scalability for industrial applications [1].

Experimental and/or Modelling: *Reagents:* Methylene Blue dye from Fluka Chemie AG, Aquasorb L24 mesh 12x40 adsorbent and distilled water were used.; *Experimental conditions:* Preliminary tests included investigation of two initial dye concentrations of 20 mg/L and respectively, 50 mg/L, at two different rotational speeds of 500 and 1000 rpm, respectively, at 20°C room temperature and 45°C, respectively.; *Analysis method:* Spectrophotometry using a Hitachi U-5100 UV-VIS Spectrophometer was applied to measure absorbance at MB characteristic wavelength of 660 nm.; *Experimental methodology*: Experiments were conducted in a batch system, with sampling every 2 or 3 minutes to measure the absorbance.

Results and discussions: High efficiency color removal, in comparison to a regular batch system, for the same working conditions, was attained. Variations in the initial adsorbent concentration exhibited significant impacts on the adsorption efficiency of the system, especially at large rotational speeds. Figure 1 showing color removal variation in time at 20°C, at two different rotational speeds of 500 and 1000 rpm, indicates effective removal rates of approximately 90% in 40 min time interval, with faster removal rates at the largest spinning speed. Experimental results obtained at 45°C, at same rotational speeds of 500 and 1000 rpm, are presented in Figure 2 and reveal 88% color removal at lower spinning speed and 94% discoloration at 1000 rpm, both after only 30 min working time period.

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Utilizing a screening process, the study examines also the impact of different parameters on color reduction, with rotational speed identified as the factor exerting the most significant influence in reducing color.

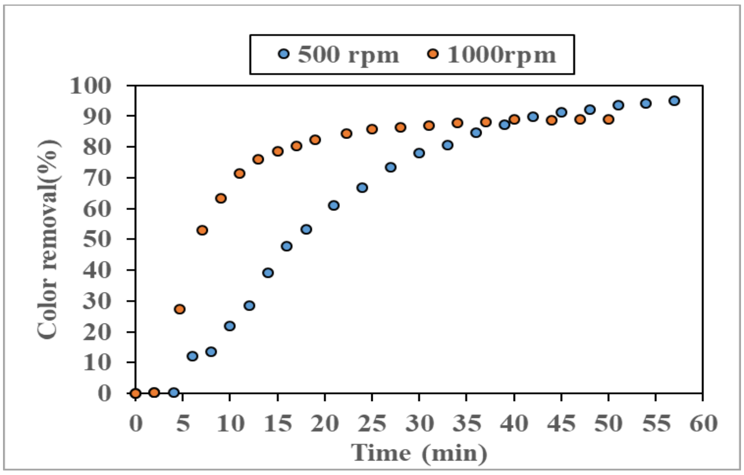

Fig. 1 MB color removal at 20° C and two different bed rotational speeds, 500 and 1000 rpm

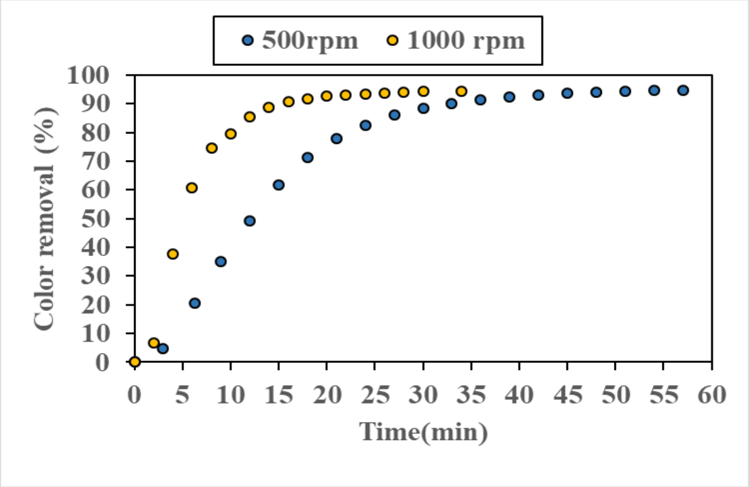

Fig. 2 MB color removal at 45° C and two different bed rotational speeds, 500 and 1000 rpm

Conclusions: The experimental data revealed a direct correlation between higher rotational speeds and elevated temperatures with increased methylene blue adsorption capacities.

References:

[1] Guo Q., Zhao Y., Liu Y.Performance and Mechanism of Gas-Solid Adsorption in a Rotating Adsorption Bed, *Chem.Eng.Tech.*, 45, 5 (2022), 844-852.

SA-P09 DEVELOPMENT OF A NOVEL TWO-COMPONENTS MATERIAL AND ITS APPLICATION AS EFFICIENT DYES ADSORBENT

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Abstract: *A new adsorbent material was synthesized and characterized. Its abilities of retaining a dye model molecule from its aqueous solution were tested and promising results were obtained.*

Key words: adsorption, cherry stones, equilibrium isotherm, kinetic studies, Response Surface Methodology

Introduction: Water is one of the vital resources for the environment and human existence. However, there is a risk to the water quality mainly because of the industrial effluents discharged without being properly treated. Produced in striking quantities and diversity over the globe [1], dyes are often listed among the reported persistent contaminants. They can cause severe toxicity and carcinogenicity, skin irritation, allergic dermatitis, cancer, and mutations [2]. As consequence, many efforts are currently focused on developing and implementing different methods of water depollution.

Experimental and/or Modelling: First and foremost, the goal of this endeavor was to produce a novel material with desirable adsorbent qualities. An inert polymer served as inclusion matrix for cherry stone powder, an underappreciated by-product of the fruit processing industry and the adsorbent was tested against a model azo dye molecule.

Results and discussions: The obtained material was analyzed by scanning electron microscopy and by Fourier-transform infrared spectroscopy. The analysis revealed that the material has a porous nature and that an appropriate incorporation of the cherry stone powder in the polymeric matrix was attained. The target dye compound was retained from its aqueous solution by the prepared product. Response Surface Methodology was utilized to optimize three factors (the initial pH of the dye solution, the amount of the added adsorbent, and the working temperature) known as having a significant influence on process development. Several isotherm and kinetic models were applied to the experimental data. The adsorption process follows Freundlich and Temkin equilibrium isotherms and is well characterized by pseudo-second-order kinetics.

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Conclusions: Based on the documented outcomes, we may infer that the manufactured product is a feasible adsorbent material because the refractory pollutant was nearly entirely eliminated from the medium.

References:

[1] Altıntıg, E., Ates, A., Angın, D., Topal, Z., Aydemir, Z., Kinetic, Equilibrium, Adsorption Mechanisms of RBBR and MG Dyes on Chitosan-Coated Montmorillonite with an Ecofriendly Approach, *Chem. Eng. Res. Des.* 188, (2022), 287–300.

[2] Chatterjee, S., Ohemeng-Boahen, G., Sewu, D.D., Osei, B.A., Woo, S.H., Improved adsorption of Congo red from aqueous solution using alkali-treated goethite impregnated chitosan hydrogel capsule. *J. Environ. Chem. Eng.* 10, (2022), 108244.

SA-P010 THIN-LAYER CONVECTIVE DRYING OF CHICKEN BREAST FILLET: EXPERIMENTAL AND MODELLING

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Abstract: *Thin-layer convective drying of chicken breast fillet was conducted under different operating conditions. The effects of process factors on its performances were quantified using a semiempirical model based on Fick's second law.*

Key words: Thin-layer drying, diffusion coefficient, Fick's second law, modelling

Introduction: Experimental determination of drying curves and their prediction by modelling are essential for the design, control, and optimization of the meat drying process [1].

Experimental and modelling: Convective drying experiments of thin-layer (7 mm) of bulk and chopped chicken breast fillet were performed at different levels of process temperature until an approximately constant mass was observed. Experimental runs were conducted in three drying devices, *i.e.*, a food dehydrator (at 70 °C), a thermobalance (at 75 °C, 85 °C, 95 °C, 105 °C, and 120 °C), and a vacuum drying oven (at 100 °C). A semiempirical model based on Fick's second law [2] was used to predict the dynamics of thin-layer drying. The adjustable parameter of the model, *i.e.*, effective diffusivity (D_{eff}), was determined from experimental data.

Results and discussion: The values of D_{eff} for chopped meat ($1.2–3.4\times10^{-10}$ m^2/s) were 20–67% higher than those for bulk meat ($1.0–1.7\times10^{-10}$ m^2/s). The values of D_{eff} in vacuum drying oven ($1.0–1.2\times10^{-10}$ m^2/s) were 20–83% lower than those in food dehydrator ($1.3–2.1\times10^{-10}$ m^2/s) and thermobalance ($1.2–3.4\times10^{-10}$ m^2/s). Moreover, for convective drying in the thermobalance, D_{eff} increased with an increase in the temperature, this increasing trend being more pronounced at operating temperatures up to 95 °C.

Conclusions: Thin-layer convective drying of chicken breast fillet was affected by operating conditions, including processing of raw material subject to drying, experimental device, and operating temperature. Chopped fillet drying in a food dehydrator or thermobalance at temperatures up to 95 °C is recommended.

References:

[1] Álvarez S., Álvarez C., Hamill R., Mullen A. M., O'Neill E., Drying dynamics of meat highlighting areas of relevance to dry-aging of beef, *Compr. Rev. Food Sci. Food Saf.*, 20, 6, (2021), 5370-5392.

[2] Stoica-Guzun A., Pârvulescu O.C., Broșteanu A., Chira N., Stroescu M., Dobre T., Influence of sea buckthorn pomace pretreatment and drying conditions on the drying kinetics, quantity and quality of seed oil, *J. Food Nutr. Res.*, 57, 4, (2018), 363-372.

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SA-P011 EFFECTIVE DIFFUSION COEFFICIENTS IN POROUS COMPOSITE MATERIALS

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Abstract: *Methods for experimental determination and mathematical modeling of diffusion processes will be applied to highlight some aspects regarding the behavior of composite materials obtained from solid waste in contact with organic vapors or humidity, simulating real conditions of use.*

Keywords: effective diffusion coefficients, construction materials, porous materials

Introduction: According to data published in literature, the construction sector is responsible for approximately 40% of the pollution produced and approximately 30% of the consumption of raw materials worldwide.

Modelling and discussions: The European Union (EU) has set itself the ambitious goal of transforming the building sector into a zero-emissions frontier by 2030. The new EU initiative requires all new buildings to achieve zero-emission status by 2030, while buildings occupied or owned by public authorities must meet this standard by 2028. Emissions assessment criteria include global warming potential per cycle life of a building, taking into account each phase in production.

For residential buildings, the EU requires a significant reduction in average primary energy consumption – by at least 16% by 2030 and by 20-22% by 2035.

This directive also provides for the renovation of the 16% most energy-inefficient non-residential buildings by 2030, expanding to 26% by 2033, by establishing minimum energy performance requirements. A significant evolution can be observed in the construction industry towards more environmentally friendly and sustainable options, these being achieved with the help of the materials used. Adding porous materials can improve the quality of building materials due to their contribution to thermal and acoustic insulation, moisture management, freeze-thaw resistance, durability, energy efficiency and aesthetic appearance of buildings.

International trends regarding the use of construction materials with different porosities may vary depending on various factors, the evolution of technology, environmental concerns and especially construction requirements.

Degradation induced by the diffusion of chemical compounds and/or moisture is a major factor that affects the durability of structures made of different construction materials. Studies on the diffusion of some components in these types of materials are very important.

Conclusions: In this study, several ways of determining the effective diffusion coefficients of some compounds, in gaseous or liquid state, in materials with homogeneous or heterogeneous mesoporous structure are investigated.

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SA-P012 RECOVERY OF Nd FROM HDD MAGNETS

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Abstract: *In this paper there is presented a way to recover Nd from REM scrap using liquid-metal extraction with molten magnesium as an extractant and a vacuum magnesium distillation process to separate the Nd from magnesium-neodymiym alloys. In the last decade, the supply of REEs has come under considerable pressure, according to EU 2020 Critical Raw Materials Resilience. Despite these facts, only around 1% of the REE are recycled from scrap [2].*

Key words: REE, neodymium, HDD, microwave, LME, vacuum magnesium distillation process

Introduction: Rare-earth elements (REE), notably neodymium, dysprosium, and praseodymium, are indispensable for green technologies such as electric vehicle motors and wind generators. To address the limited supply and processing complexity, recycling rare-earth magnets has become crucial. Despite supply pressures, only about 1% of REE is currently recycled.[1-3]

Experimental: REE permanent magnets (Nd: 20-23 wt.%, Dy: 1-7 wt.%, Pr: 0.5-6 wt.%) were manually dismantled from PC-HDD voice coil motors, crushed, and subjected to liquid metal extraction (LME) in a microwave (MW) furnace using molten Mg as the extractant [3]. The separation of REE from obtained Mg-REE alloys was investigated via vacuum magnesium distillation process (figure 1) [4]. Various experimental parameters were examined in order to establish the optimal Nd extraction conditions.

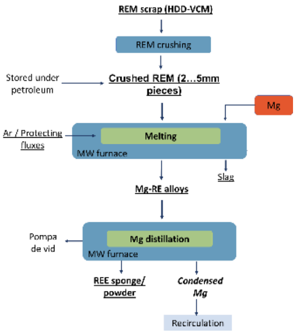

Figure 1. Flowsheet for recovery of Nd from HDD magnets

Results and discussions: The Nd content in Mg alloy increased with increasing temperature and holding time.

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At a temperature of 800°C, a duration of 8 h, a granulation of the magnets of 2-5mm, using a LiF-LiCl-MgF_2 protecting flux and furnace Ar atmosphere, the Nd content was 45wt.% and the extraction yield of >90%.

When separating Nd from the alloy by vacuum distillation, at temperatures of 850-900 for 8 hours, a Nd sponge with a content of > 98% Nd was obtained.

Conclusions: This study demonstrates that liquid metal extraction using molten Mg, followed by a vacuum distillation process, carried out in a MW furnace, could be a viable method for recovery of the expensive rare earth element Nd from NdFeB permanent magnets scraps. The effects of Mg/REE ratio, temperature, holding time, scrap sizes and protecting fluxes composition on extraction behaviour of the Nd from Nd-Fe-B magnet scraps were investigated.

Acknowledgements: This work was supported in the frame of the COFUND-ERAMIN-3-MW4REMAM-2, Project ID 387, Contract 309, financed by UEFISCDI.

References:

[1] 1. K. Binnemans et.al., *Nature Reviews Materials* 6, (2021) 459
[2] L. Nickels, *Metal Powder Report* 75 (2020) 189
[3] S. Park, et.al., *Arch. Metall. Mater*. 65 (4) (2020) 1281
[4] M.Z. Rasheed, et.al., *Metallurgical and Materials Transactions* 52B (2021) 1213

SA-P13 THE EFFECT OF ACID TO NATURAL GAS STORAGE ROCKS

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Abstract: *Natural gas deposits are energy reservoirs of great importance in providing transitional fuel for a future without harmful emissions for the environment and humanity. However, the productive layers within the gas deposits are characterized by the porous and sealing environment, and the flow of natural gas and associated fluids is complex, productivity being dependent on the movement of fluids through the rock pores and associated phenomena. Exploiting gas deposits located in shale (clays) has brought new challenges in studying their productivity dynamics, with very low permeability being an essential factor in obtaining economic flows. That is precisely why hydraulic fracturing is widely used in the exploitation of natural gas deposits, the role of this technique being to increase the production of natural gas, primarily from unconventional deposits (shale and clay).*

Key words: *natural gas, acid, rocks*

Introduction: About 85% of the world's shale gas wells are drilled through vertical and horizontal wells, from which fissures (crevices) are then developed through multiple fracturing.,This constant temperature maintenance means that the natural gas is extracted in the state of gas aggregation without being affected by its passage into the biphasic phase. However, both during the exploitation period (when the water associated with the deposit and especially the well condensate) and during their ascent through the extraction pipes, the temperature changes, and then the condensation of wet gases or even the engagement of liquid fractions in the pores of the productive rocks occurs, leading to a decrease in the amount of extracted gas. These problems (decrease in the productivity of gas wells, penetration of liquid water into treatment facilities, appearance of cryohydrates, accumulation of liquid in the area of extraction wells) lead to significant economic losses.

Experimental and/or Modelling: In this material we discussed the effect of acidification on the increase of the natural gas recovery factor.

We have found that the complete process of neutralizing hydrochloric acid is 30-50 minutes for limestone and 30-90 minutes for liming with 10-12% SO_4Ca.

The speed of neutralization of the acid is a function of the quantity and quality of the acid used per surface unit, in the analysis carried out on some calcareous rocks from the gas exploitation in the Mediaș area, we found that we can use a relationship of the type, in establishing the neutralization time of the acid:

$$t=Kd+c$$

Where:

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-t is the duration of neutralization, minutes,
-d represents the channel diameter, cm,
-K is an acid neutralization coefficient,
-c is a correction coefficient of the equation.

We also found, on the data obtained experimentally, that the logarithmic equations of the decrease in the concentration of the solution as a function of the reaction time between hydrochloric acid (HCl) and rock have the lower error coefficient, a and b being the correction parameters depending on the concentration in $CaCO_3$.

$$t=a \ln(d)+b$$

Conclusions: In this study we analyzed the influence of the temperature of the productive layer and/or of the acid solution, noting that by raising the temperature of the acid solution, the rate of reaction between HCl and rock increases.

In industrial practice, the acidification of productive layers is carried out with acid solutions of concentration between 8 and 15%.

Using a solution with a lower concentration requires large amounts of liquid and also cracking occurs only over short distances, and in the case of a higher concentration, it will lead to the formation of viscous solutions consisting of $CaCl_2$ and $MgCl_2$, sometimes even leading to pore blocking.

Also, during the chemical reaction, it can appear as a CO_2 product, which can be in the form of gas or (under the action of pressure from the productive layers) can dissolve in water.

The release of CO_2 from the solution will cause the solution to bubble and therefore some reaction products will separate more quickly.

References:

[1] Zeinab A., Pozo A.O., Claudia Maria Brezeanu M.C., Chis T. (2023) *Novel acid soluble abrasive material for abrasive jet perforation through coiled tubing and ts-tool for carbonate gas well – Yard test*, Romanian Journal of Petroleum & Gas Technology VOL. IV (LXXV) • No. 2/2023, pp. 97-108, DOI: 10.51865/JPGT.2023.02.10, http://jpgt.upg-ploiesti.ro/wp-content/uploads/2023/09/10_RJPGT_2023-timur-chis-4-final.pdf,

SA-P14 WATER SEPARATION IN NATURAL GAS PIPELINES

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Abstract: *Multiphase flow can be defined as the simultaneous flow of several phases or the flow through a defined surface of a flow consisting of the two (three) phases (liquid, solid, gas) interacting or moving (sliding) independently, one next to the other. The study of multiphase flow is critical in the energy industry, especially in oil and gas extraction. The transport of two-phase gas-liquid mixtures through horizontal, vertical, or inclined pipelines is encountered in the crude oil extraction industry, industrial processes in chemical reactors, the flow of fluids through heat exchangers, and even in cooling/condensing processes. That is why, in this material, we describe a new technique for analyzing the separation of water in the gas flow.*

Key words: *Multiphasic separation, natural gas*

Introduction: The water content of natural gas depends on the state parameters; above specific values, the water is in the liquid phase. Its existence in the liquid phase leads to transport difficulties and other deficiencies (corrosion, reduction of caloric capacities, etc.). The separation of water by mechanical methods must be considered in that the lengths of the transport systems are appreciable, and these correctly chosen methods can be effective for an extended period. Apart from these considerations, the mechanical methods also have the advantage of using the energy of the transported gases. The water finely dispersed in the mass of gases is transported along the pipeline, and the force that achieves this transport is called the forward resistance force. This force, denoted F_R, for a sphere with diameter d_p, is calculated using the classical relation.

$$\boldsymbol{F_R = C_D \frac{\pi d_p^2}{4} \frac{1}{2} \rho v^2,}$$

where the resistance coefficient C_d is determined by one of the relationships given in [1,2]:

$$C_D = \frac{24}{Re_p} \text{ pentru } Re_p < 2;$$

$$C_D = \frac{18}{Re_p^{0,6}} \text{ pentru } 2 \le Re_p < 200;$$

$$C_D = \frac{24}{Re_p}\left(1 + \frac{0,15}{Re_p^{0,687}}\right) \text{ for } 200 \le Re_p \le 800;$$

$$C_D = 0,44 \text{ for } 800 < Re_p.$$

The Reynolds number for the particle, Re_p, is defined by the mean relative velocity $(v - v_p)$ and the particle diameter d_p obviously, at a relatively zero speed $v - v_p = 0$, the forward resistance has zero value. It is easy to establish that the difference

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between the velocity of the gas v which is assumed to be fixed for a given situation and the velocity of the particle v_p is always positive and in this way the Reynolds number for the particle is

$$Re_p = \frac{\rho(v - v_p)d_p}{\mu} = \frac{\rho v d_p}{\mu}\left(1 - \frac{v_p}{v}\right) = \frac{\rho v d}{\mu}k(1 - \varepsilon)$$

where the notations were used: $k = \frac{d_p}{d}$, $\varepsilon = \frac{v_p}{v}$, d being the inner diameter of the pipe and taking only positive values.

Experimental and/or Modelling: It is possible to obtain a correlation between the thickness of the water film and the length of the surface of the separator, which, as we specified, we now admit as being formed by a flat surface inclined to the horizontal plane with an angle α. The flow equation is the starting point for obtaining this dependence, which means that in the elementary time interval *dt:*

$$\boldsymbol{dV = dQ \cdot dt = \left(\frac{\rho_a g \sin\alpha}{\mu_a} h^2 - \frac{\tau_a}{\mu_a} h\right) dhdt,}$$

where h represents the thickness of the water film as a function of x. On the other hand, also during the elementary time dt, the gas stream entrains a volume of water equal to

$$dV = v_m(1 - e)\cos\alpha dxdt,$$

where v_m is the average speed of the gas stream, and *e* is specified, the fraction of water expressed under the conditions of pressure and temperature at which water separation is achieved.

The differential equation results from the equality of the two elementary volumes

$$\frac{\rho_a g \sin\alpha}{\mu_a} h^2 dh - \frac{\tau_a}{\mu_a} hdh = v_m(1 - e)dx.$$

If we use the boundary conditions

at *x*=0, *h*=0 and *x*=*l*, *h*=*h*

results in the variation of the thickness of the water film h depending on the length l of the plate

$$\frac{\rho_a g \sin\alpha}{3\mu_a} H^3 - \frac{\tau_a}{2\mu_a} H^2 = v_m(1 - e)\cos\alpha \cdot l,$$

which shows that the thickness of the film varies with the parameters v_m, *e* and the length of the separator surface l.

Conclusions: The water film collected by the surface of the separator increases its thickness depending on the free water from the transported gases.

References:

[1] Robescu, D.N., Szabolcz, L., Robescu, L.D., Constantinescu, I., Dinamica fluidelor polifazate, Editura Tehnică, Bucureşti, 2000.

SA-P15 USE OF HYDROGEN MIXED WITH NATURAL GAS IN INDUSTRIAL AND LOCAL NETWORKS

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Abstract: *Hydrogen gas pipelines are technically feasible and have operated for decades in various locations, including the US, Germany, the Netherlands, France, and Belgium.*

However, the scale of these pipeline systems is quite limited, and they need to provide an extensive basis for the modernization and rapid growth of the implementation of new hydrogen transport systems. In some parts of the world, significant infrastructure exists for transporting and distributing natural gas. Such infrastructure can facilitate low-cost transportation, distribution, supply, and hydrogen storage. The article presents the natural gas-hydrogen blending projects in Europe under study.

Key words: Natural gas, hydrogen, blending

Introduction: The realization of hydrogen-compatible gas transport networks involves a series of adaptations and problems to be addressed and solved for each of their components, which include the transport and distribution network and storage and utilization facilities. Several important elements regarding the gas network are the material from which the pipe is made, polyethylene vs. steel, compressors, regulating, measuring, and safety equipment, and mixture levels, all of which must be adjusted to transport a mixture of hydrogen and natural gas.

Experimental and/or Modelling: A recent study in the Netherlands concludes that its gas pipelines can be converted for hydrogen gas by replacing gas compressors and seals. Likewise, in Great Britain, detailed studies are conducted, which take into account the fragility of the current high-pressure natural gas transport pipelines if they will transport pure hydrogen and the changes that must be made to the operating and safety regulations. The presence of hydrogen in the existing natural gas pipelines will cause their walls to be much more strongly influenced by the demands to which they are subjected. The phenomenon is closely related to pressure variations in the pipelines and is essential to analyze and comply with over time. Research has so far shown that this phenomenon of hydrogen embrittlement does not have as great an influence as originally thought, and the process of transporting hydrogen through the existing pipeline system can be carried out safely and reliably [1]. Currently, acceptable hydrogen mixture volumes of 10 vol.%, 15 vol.%, or values up to a maximum of 30 vol.%, are considered feasible for certain appliances, stoves, and boilers used in local applications.

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Results and discussions: The transformation of natural gas into hydrogen through gas reforming with carbon dioxide capture and sequestration and the transformation of renewable energy into hydrogen through electrolysis allow energy consumers to obtain cost reductions, only if the existing natural gas infrastructure is used. In the case of used pipelines, as is the case of pipelines in Romania that have exceeded their service life, they are susceptible to being in the critical zone, it is necessary that the hydrogen tolerance be checked individually, and in the case of critical results, to be specified method of intervention.Several projects around the world have demonstrated that at 20 vol% hydrogen the existing gas network does not require much modification and the effect of the mixture on materials in the short term is not to be worried about. What has yet to be proven is the long-term effect this mixture of hydrogen and natural gas has on materials and equipment, complicating planning for large-scale blends by industry utilities [2].

Conclusion: It has been demonstrated in the specialized literature that the impact on some gas quality criteria related to combustion (relative density, net and gross calorific values and the Wobbe index), of the mixture of gases and hydrogen, changes as follows:

- As the hydrogen concentration increases, the calorific value decreases linearly. Compared to methane, the lower calorific value and higher calorific value for pure hydrogen decrease to 30% and 32%, respectively;
- The relative density of hydrogen is about eight times lower than that of methane, this results in the change in the Wobbe index, the decrease from pure methane to pure hydrogen is less severe, as the change in calorific value is largely counteracted by the change in densities.

The difference in Wobbe indices between CH_4 and H_2 is only about 9.5%, while the change in calorific value is about 68%.

- The Wobbe index does not decrease over the entire range of mixture space, instead it actually increases with increasing hydrogen concentrations for very high hydrogen fuel mixtures.

References:

[1] https://cdn.wwf.ro/uploads/2023/01/26162703/WWF-Romania-si-Bankwatch_Analiza-Hidrogen.pdf

[2] http://stiintasiinginerie.ro/wp-content/uploads/2014/01/16-ANALIZA-DIFERITELOR-METODE-DE-OB%C5%A2INERE.pdf

SA-P16 CHEMICAL INTERCATION OF NATURAL GAS TO SALINE CAVES STORAGES

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Abstract: *Natural gas represents that energy potential that can be stored in large quantities, in the same state in which it is used by the final consumer, without being subjected to transformations and interruptions. One of the fundamental problems of any gas industry is taking over hourly and seasonal consumption peaks, caused by the random nature of gas demand, depending on the nature of the consumers (industrial with a relative constancy and non-industrial, mainly households, with large hourly and seasonal fluctuations) and import possibilities, with approximately uniform and limited capacities, during a day or the entire cold season. This paper presenting a gas storage in salt cave.*

Key words: natural gas, storage, salt

Introduction: The underground gas storage thus appears as a requirement for

a) providing gas to consumers in case of damage to large gas pipelines, by temporarily replacing gas sources;

b) the standardization of the importation of natural gas over the course of a year with direct consequences on their purchase prices and the attractiveness of the contracts;

c) covering consumption peaks in the cold season, by compensating the gas flows necessary for heating;

d) the transfer of gases from fields with a high dynamic potential to underground deposits located near large consumers;

e) the standardization of mechanical demands and the transport capacity of gas pipelines between sources and consumption areas;

f) a special strategic role, a fact for which the European Directives require the existence of storage capacities from which to ensure the supply of natural gas to the domestic market for a period of between 90 and 120 days.

The storage of natural gas (in underground or above-ground tanks) represents an efficient process that combines the constant supply of natural gas, through transport pipes, with the variable demands of the market, which depend on the weather or economic considerations. During the summer, when the transport capacity of the pipelines far exceeds the demand for consumption, natural gas is stored to be extracted most often in the winter, when gas consumption increases greatly, or depending on the economic considerations of that period . Seasonal consumption peaks can be covered by underground gas storage in warehouses located near large consumption centers.Salt caverns are sealed against salt due to its unique properties.

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In addition, salt pillars of large widths and thicknesses positioned above and below the cavern, which are necessary for the mechanical stability of the host rocks, combine this tightness with the thick layers of sealing salt. Salt deposits can be structured into salt domes, salt diapirs and layered salt. Depending on its appearance, the salt may be contaminated, but generally this will not affect its tightness. The applicable storage pressures depend on the depth of the cavern, the operational scheme and vary approximately between 30 and 80% of the lithostatic pressure of the rocks. At a common cavern depth of 1,000 m, this corresponds to a maximum pressure of about 180 bar and a minimum pressure of about 65 bar.

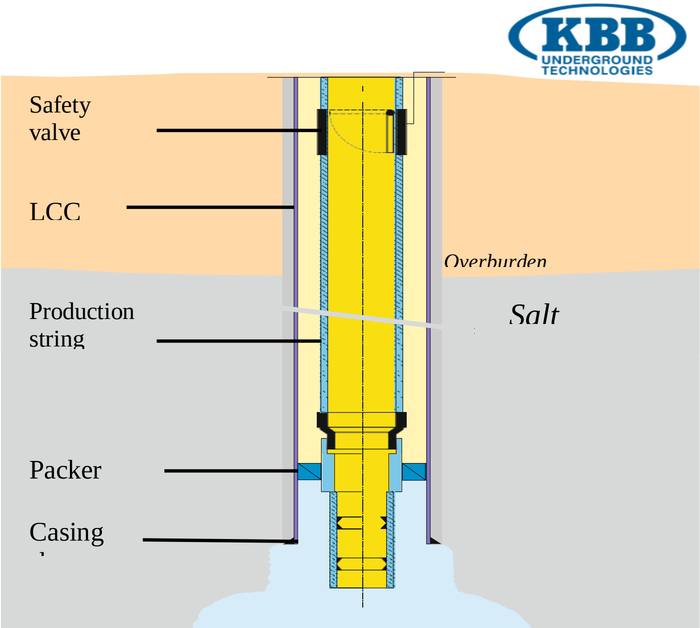

Fig. 1. Gas cavernes

Conclusions: In the process of determining the shape and dimensions of the cavern for natural gas storage, hypotheses are used. The thickness of the salt formation is assumed to satisfy the necessary requirements for gas storage and the width and length of the salt formation are considered finite in relation to the diameter of the salt cavern. The salt formation is considered a visco-elastic, isotropic material because it is composed of a relatively homogeneous material (especially NaCl).

Due to the failure mechanisms of the cavern, the upper and lower structures are very different from each other, the mathematical models of the two parts are built separately in sections.

References:

[1] Ikoku, C., U., - Natural Gas Production Engineering, New York: John Wiley & Sons Inc., 1984,

SA-P17 LABORATORY ANALYSIS OF OILFIELD PRODUCED WATER EXTRACTION FROM EMULSIONS, PETROLEUM ENGINEERING ENHANCED OIL RECOVERY

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Abstract: *The water connected dangers in the refining, oil exploration, and dissemination are deliberated. Subsequently the oil produces deliver completed 90% of transportation liveliness in practically all republics, oil source interjects might have thoughtful belongings, not individual on movement, but correspondingly on the food distribution and manufacture, medical care, heating, manufacturing, national security, and other energetic occupations of the contemporary societies. Once oil is discovered in the water uncommon areas the water possessions developed harassed. Off-shore oil examination generates risks for the maritime lifecycle while oil dissemination and transportation determination produce cumulative risk for the ecosystem in case of accidents or leakages. The petroleum manufacturing commonly categorizes the crude oil through the geographic position it is fashioned in, its thickness, and its sulfur contented. A heavy crude oil has a high density and a light crude oil has a stumpy thickness. An oil well products principally crude oil, through some natural gas softened in it. Since the compression is subordinate at the surface than underground, selected of the gas will originate out of solution and will be either burned or healthier. Crude oil is also found in semi-solid form mixed with sand and water, as in the Athabasca oil sands in Canada, anywhere it is frequently mentioned to as the crude bitumen. Bitumen is a black, sticky, tar-like procedure of the crude oil which is so heavy and thick that it obligation be impassioned or thinned beforehand it determination flow. In the study on water source quality, the particle size and suspended solid concentrations and oil content in water source are mainly considered.*

Key words: Oil field, water

Introduction: The Natural gas hydrate in the underwater mainland permafrost and boundaries coatings have been documented as an eccentric natural gas reserve. In this approaches of hydrate sediments gas production, like thermal stimulation, depressurization, and combination chemical inhibitor stimulation of these methods, percolation possessions regulator fluid flow in hydrate residues through chemical transfer and heat. The permeability importance throughout the gas production has led to widespread examines of relative permeability and absolute in the hydrate sediments. Certain industrialized a numerical prototypical to examine the belongings of various arguments, like absolute, permeability reduction index, and relative permeability, and porosity, throughout the gas production from porous media comprising hydrates. The datasets showed diminishing the grain size and permeability decrease proponent increased the rate of hydrate dissociation. Fig 1

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indicates that big enough particle size of suspended solid in injected water might cause rock permeability loss.

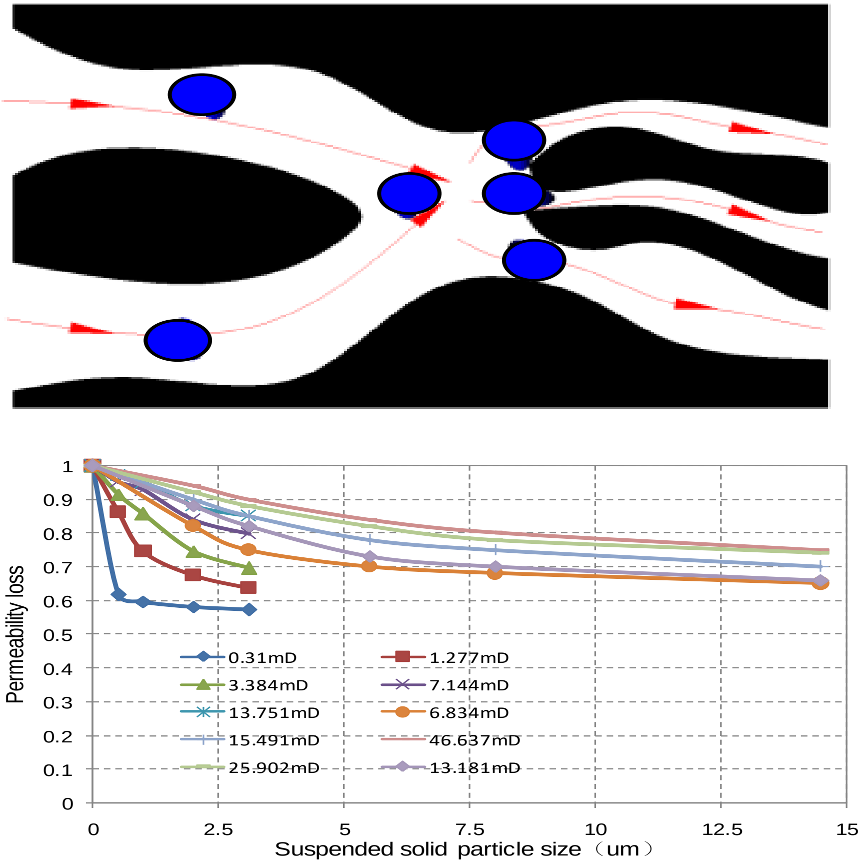

Fig. 1. Core permeability loss vs. suspended particle sizes

Conclusions: This recommended that the permeability reduction index and comparative permeability model, which were created on the changed hydrate formation types in the porous media, were of great prominence for approximating the gas production.

References:

[1] *Reem Sabah Nohammad, Daniel Iancu, Doru Stoianovici, Timur Chis*, Neuronal modeling of water properties on oil field**,** SICHEM 2022, Book of Abstract, ISSN 2537-2254, 17-18 November, 2022,

SA-P18 ASPHALTENES DEPOSITION MODELING IN CRUDE OIL, A COMPARISON TO CHOLESTEROL DEPOSITION MODEL IN ARTHERIES

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Abstract: *Asphaltene deposition from Crude Oils has always posed challenges as it created serious technological issues with devastating consequences in crude oil reservoirs, production wells, crude oil floating storage units and crude oil magistral pipelines if the amount precipitated is large. This fact is attributed to the amount of asphaltene found in most of the crude oils' existent on the market, each one-with a demonstrated potential for aggregation, flocculation, precipitation and deposition along the extraction, storage, and transportation phase [1]. Although the mechanism of asphaltene deposition has been given an ample consideration throughout studies, most of them have addressed only partially the mechanism and its deposition behavior due to the numerous factors involved and complexity of the components of crude oil and processes involved [2,3]. That is why, recent studies are trying a different approach based on a more fundamental model with relations to the ones found in nature, not necessarily linked to hydrocarbon fractions, but one which shows many similarities in the deposition model [4]. Thus, in this paper, we are presenting the similarities of the Asphaltene Deposition Model on the inner wall of Pipelines with the Cholesterol Deposition Model on the Arteries, analyzing possible causes why Asphaltenes tend to aggregate and clog only specific areas of the installation and not globally, due to a combination of turbulent flow, wall shear stress [WSS] and concentration of the asphaltenes in its different forms through the stream.*

References:

[1] Sherif Fakher, Mohamed Ahdaya, Mukhtar Elturki, Abdulmohsin Imqam, Critical review of asphaltene properties and factors impacting its stability in crude oil, Journal of Petroleum Exploration and Production Technology (2020) 10:1183–1200

[2] D. Eskin, J. Ratulowski, K. Akbarzadeh and S. Pan: Modelling Asphaltene Deposition In Turbulent, Pipeline Flows, Schlumberger DBR Technology Center, Edmonton, AB, Canada T6N 1M9

[3] Peyman Kor, Riyaz Kharrat b: Modeling of asphaltene particle deposition from turbulent oil flow in tubing: Model validation and a parametric study, Petroleum 2 (2016) 393-398

[4] Myriam Cilla, Estefanía Peña, and Miguel A. Martínez: Mathematical modelling of atheroma plaque formation and development in coronary arteries, J R Soc, 11(90); 2014

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SA-P19 PREDICTION OF THE DYNAMICS OF UREA AND CREATININE CONCENTRATIONS IN RENAL DIALYSIS PROCESS

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Abstract: *Dynamics of urea and creatinine concentrations in blood and dialysate were predicted by assuming an analogy between the mass transfer through a tubular membrane and heat transfer through the wall of a coil immersed in a perfectly mixed liquid.*

Key words: dialysis, heat transfer, mass transfer, modelling

Introduction: In a classic kidney dialysis facility, the blood with high concentrations of urea (u) and creatinine (c) flows through a tubular membrane immersed in the dialysis solution (dialysate), which is under agitation. Mass transfer of species $j=u$, c from the blood to the dialysate occurs through the membrane, resulting in a decrease in the concentration of species j in the blood.

Experimental and modelling: An analogy was assumed between the mass transfer through a tubular membrane immersed in a perfectly mixed dialysate and the cooling of a warm liquid flowing through a coil immersed in a perfectly mixed cold liquid [1,2]. Simple analytical equations were determined to predict the dynamics of species concentrations in blood (c_{j1}) and dialysate (c_{j2}), as well as the mass of species j transferred from blood to dialysate ($m_{j,transf}$), considering a constant volume of dialysate (V_2). Dynamics of c_{j2} and $m_{j,transf}$ were simulated at different values of V_2 (5–25 L). The following levels of process parameters were considered for dialysis simulation through a hollow fiber membrane (1 mm diameter, 0.1 mm wall thickness, and 5 m^2 transfer surface area): a blood flow rate of 0.2 L/min, initial concentrations of urea and creatinine in blood of 1000 mg/L and 40 mg/L, respectively, and in dialysate of 0 mg/L. The simulations indicated that c_{j2} decreased with V_2, $m_{j,transf}$ increased with V_2, and for a dialysate volume V_2=20 L, the concentrations of species j in blood decreased from the initial value to a normal value after 25 min.

Conclusions: Dynamics of urea and creatinine concentrations in blood and dialysate were predicted using analytical equations determined by assuming an analogy between the mass transfer through a tubular membrane and heat transfer through the wall of a coil immersed in a perfectly mixed liquid. Based on these equations, relevant dialysis factors can be controlled and optimized.

References:

[1] Bratu E. A., *Unit Operations for Chemical Engineering*, Technical Book, Bucharest, 1983.

[2] Thews O., Hutten H., A comprehensive model of the dynamic exchanges during hemodialysis, *Med. Progr. Technol.*, 16, 3, (1990), 145-161.

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SA-P20 THE APPLICATION OF RHEOVISCOSIMETRY IN THE STUDY OF SUBSTRATES HYDROLYSIS WITH SPECIFIC DRUGS - PART II

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Abstract: *The ability to hydrolyze proteins of some specific drugs (Triferment, Colebil etc.), was studied in an experimental investigation to determine, for a specific biopolymer solution with drugs content, the relationship between viscosity and hydrolysis degree of biopolymer. We determined that, by administering pancreatin the function of the pancreatic enzyme can be replaced, achieving hydrolysis as in the case of a healthy pancreas.*

Key words: enzymatic hydrolysis, viscosity, Bingham fluid, digestive enzymes.

Introduction: Nutrients from human diet are composed of carbohydrates, and proteins that are soluble in water and of fats, along with minerals and vitamins. Each requires specific, distinct pathways for digestion aiming for absorption. The mechanism of action of pancreatic enzymes (lipases, proteases, and amylases) involves the catalysis of the hydrolysis of fats to monoglyceride, glycerol and free fatty acids, proteins into peptides and amino acids, and starches into dextrin and short chain sugars such as maltose and maltriose, acting like digestive enzymes physiologically secreted by the pancreas [1-3].

Experimental *Reagents:* Starch, hydrochloric acid (Merck Germany) 1N solution, NaOH pellets, Merck, (Germany) 1N solution, NaCl (Merck Germany) 1% solution, Triferment 275 mg – tablets.

Procedure: The experimental rheological measurements, given the share rate state of versus deformation rate, was made for investigated cases, as it is shown by figure 1. The basic paper objectives consist in identification of kinetic parameters characteristizing the substrates hydrolysis when it uses as enzyme support the *Triferment* 275 mg with 8% starch solution.

Results and discussions: Figure 1 shows shear stress *vs* shear rate diagrams associated with the experimental measurements made in the case of some starch solutions hydrolysis.

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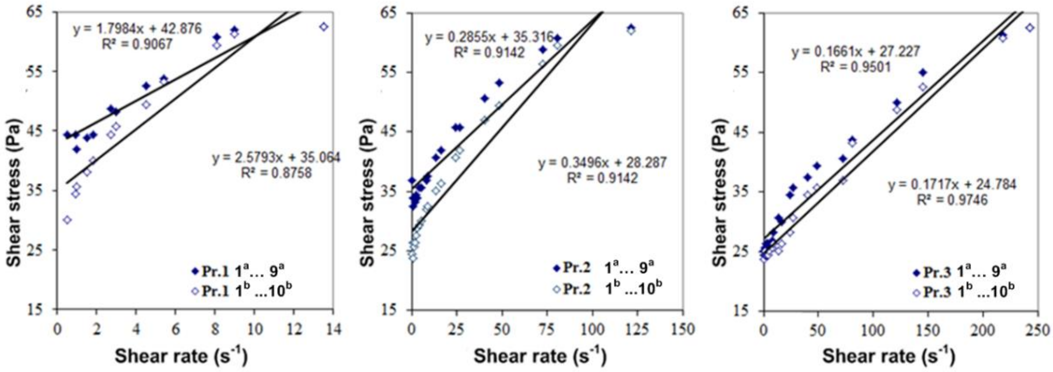

Fig. 1. Stress-strain diagrams for the starch solution after preparation, in an acidic environment (pH = 2) and in a gastric environment (pH = 2 and NaCl)

It observes that figure 1 established that starch hydrolysis, with Triferment added, is caused by the acid environment and it is very clearly seen as viscosity. So, this decreases from 1.7894 Pa·s to 0.285 Pa·s at pH = 2 and to 0.1634 Pa·s in the gastric environment. The addition of *Triferment* in the gastric medium no longer leads to the continuation of the hydrolysis or that the hydrolysis was already completed because of the previous processing of the solution. Keeping the solution processed according to the algorithm mentioned above, in gastric medium, does not make the hydrolysis progress.

Conclusions: We determined the mode of action of the enzymes on an organism whose pancreas no longer functions within normal limits, and by administering pancreatin the function of the pancreatic enzyme is replaced.

The results of this experiment showed that by taking the drug *Triferment,* enzyme hydrolysis is achieved as in the case of a healthy pancreas.

References:

[1] Netter F.H. et al., The Netter Collection of Medical Illustrations Digestive System: part II - Lower Digestive Tract, volume 9, second ed., Elsevier, 2017, ISBN: 978-1-4557-7391-6.

[2] https://pillintrip.com/medicine/triferment#desc_13, accessed December 2023.

[3] Kristó K., Bajdik J., Pintye-Hódi K., Optimization of the formulation of solid multiparticulate dosage forms containing pancreatin; *Chemical Engineering Research and Design*, 88, (2010), 1033-1036.

SA-P21 ASPHALTENES DEPOSITION MODELING IN CRUDE OIL RESERVOIRS BY COLLOIDAL AGGLOMERATION

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Abstract: *For many years, asphaltenes deposition prevention in Crude Oils have raised a heavy challenge that research is still struggling to solve. Up to present time, the deposition of asphaltenes was not a matter of if, but when and how much. Previous studies were based on thermodynamic models of solubility and colloidal to predict asphaltene precipitation.*

These models are implying that asphaltenes will precipitate from the Crude Oil into aggregates (large particles) and kept suspended by resins (which act as peptizing agents) as steric colloid. The stability of the colloid formed is a function of concentration of the resin in Crude Oil, the fraction of the asphaltenes surface sites occupied by the resins and the equilibrium conditions between the resins and on the surface of asphaltenes. The amount of resins absorbed is primarily a function of its concentration in the oil.

In this study, we have gathered on site data from several Crude Oil Reservoirs Sites during a specific period and have used the obtained data via the colloidal deposition model existing in literature in order to propose new key variables that would better describe the colloidal model deposition behavior, aiding with the better understanding of the process and shifting the target towards prevention.

References:

[1] Aboozar Soleymanzadeh, Mohammad Yousefi, Shahin Kord, Omid Mohammadzadeh: A review on methods of determining onset of asphaltene precipitation, Journal of Petroleum Exploration and Production Technology, Aug.2018

[2] Zeeshan Rashid, Cecilia Devi Wilfred, Nirmala Gnanasundaram, Appusamy Arunagiri, Thanabalan Murugesan: A comprehensive review on the recent advances on the petroleum asphaltene aggregation, Journal of Petroleum, Science and Engineering, 176 (2019) 249-268

[3] Ruiying Xiong, Jixiang Guo, Wyclif Kiyingi, Hengshui Feng. Tongcheng Sun, Xiaohui Yang, and Qing Li: Method for Judging the Stability of Asphaltenes in Crude Oil, ACS Omega. 2020 Sep 1; 5(34): 21420–21427.

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SA-P22 MODELLING OF MASS AND HEAT TRANSFER PROCESSES OCCURRING DURING THE STORAGE OF DRIED LEAVES OF *ALLIUM URSINUM*

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Abstract: *The study of the effects of air relative humidity and temperature in a warehouse on the moisture and volatile compound contents of dried medicinal plants is essential for maintaining a high quality of dried products. This research aimed at modelling the mass transfer of water and volatile compounds as well as the heat transfer that occur during the storage period of dried leaves of Allium ursinum.*

Key words: *Allium ursinum*, heat transfer, mass transfer, modelling

Introduction: The leaves of *Allium ursinum* (wild garlic, ramsons, buckrams, wood garlic, broad-leaved garlic, bear leek, bear's garlic) have multiple beneficial effects on health, *e.g.*, anthelmintic, antiasthmatic, anticholesterolemic, antiseptic, antispasmodic, cholagogue, depurative, diaphoretic, diuretic, expectorant, febrifuge, hypotensive, stimulant, tonic, vasodilator [1,2]. The research aimed at modelling the transfer processes occurring during the storage period of dried leaves of *Allium ursinum* in a warehouse, *i.e.*, (i) mass transfer of water vapour from air in the warehouse to dried leaves, (ii) mass transfer of volatile compounds from dried leaves to air in the warehouse, and (iii) heat transfer between air in the warehouse and dried leaves.

Experimental and modelling: The leaves were processed according to the technological scheme presented in Figure 1. The dried leaves were stored in Kraft paper bags that were lined with 0.3 mm polyethylene (PE) film. The bags were stored in a warehouse, where the air parameters, *i.e.*, temperature, dew point temperature, and relative humidity were measured using an EL-USB-TC-LCD data logger. The moisture content of the stored leaf samples was measured every two days. Modelling of mass and heat transfer processes was based on the following simplifying assumptions [3]: (i) perfectly mixed air in the warehouse and bag; (ii) the resistance to mass transfer of water vapour and volatile compounds to/from the bag is concentrated in the PE film; (iii) the dried leaves and air in the bag have the

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same temperature; (iv) interfacial equilibrium of the water on the surface of the dried leaf is reached very quickly; (v) the bag has a cylindrical shape.

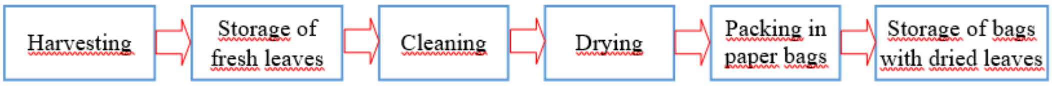

Fig. 1. Scheme of the main operations used to prepare the leaves of *Allium ursinum* for storage.

Results and discussions: Experimental and predicted dynamics of moisture content of dried leaves of *Allium ursinum* are shown in Figure 2. Air temperature and relative humidity in the warehouse increased in time, resulting in an increase in the moisture content of the dried leaves. Experimental and predicted data were in a good agreement.

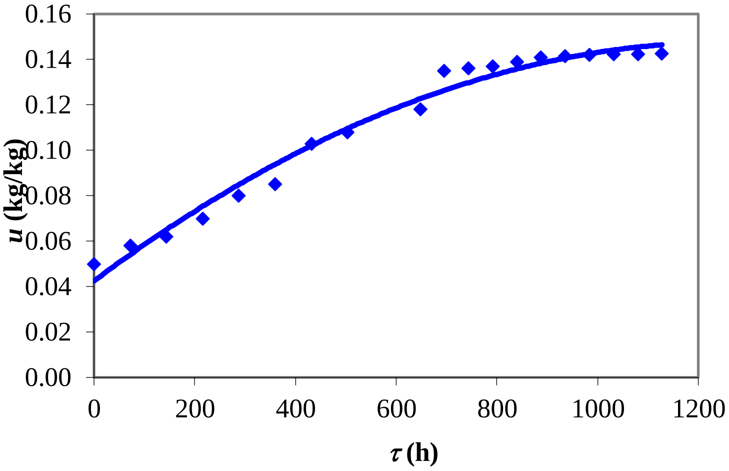

Fig. 2. Dynamics of moisture content of dried leaves of *Allium ursinum* (bullets: experimental, line: predicted).

Conclusions: Dynamics of moisture and volatile compound contents of dried leaves of *Allium ursinum* were predicted using a deterministic model based on equations of mass and heat transfer between the perfectly mixed air in the warehouse and the kraft paper bags containing the leaves. Based on this model, air relative humidity and temperature could be controlled to maintain a high quality of the dried product.

References:

[1] Sobolewska D., Podolak I., Makowska-Was, J., *Allium ursinum*: botanical, phytochemical and pharmacological overview, *Phytochem. Rev.*, 14, 1, (2015), 81-97.

[2] Tomšik A., Mastilović J., Kevrešan Ž., Vidović S., Shelf life of ramsons (*Allium ursinum* L.) under different storing conditions, *III International Congress "Food Technology, Quality and Safety"*, Novi Sad, October 2016, 531-535.

[3] Defraeye T., Verboven P., Ho Q. T., Nicolai B., Convective heat and mass exchange predictions at leaf surfaces: Applications, methods and perspectives, *Comput. Electron. Agric.*, 96, (2013), 180-201.

SA-P23 REMOVAL OF AMMONIUM COMPOUNDS FROM NATURAL SOURCES OF WATER

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Abstract: *The composition of ground water used for drinking water production is very varied. Most of the ground water sources, especially from agricultural area, contain ammonium, over maximum admissible limit. Ammonia can cause odor and taste problems, compromising disinfection efficiency by increasing the oxidant demand [WSA, 2012, E. Okoniewska,et al. 2007]. In accordance with the 2020/2184 Directive, the drinking water industry must develop new treatment methods, economical, and more effective, that should provide water of high quality and in adequate amounts. Usually, for removal of their compounds there are used physical and chemical methods like: oxidation (with air, ozon,* $KMnO_{4,}$ *clorine, hypoclorine, etc.), adsorption and ionic exchange (on active carbon, biosorbents, natural and synthetic zeolite), membranous processes (microfiltration, reverse osmosis, liquid membrane, etc.) (A.G. Tekerlekopoulou, and D.V. Vayenas, 2007, S. Edwards, et al., 2011, A.G. Tekerlekopoulou et al., 2013). It is desired for low-cost, chemically inert, natural compounds to be used in water treatment processes that do not introduce nano-, micro-particles and new compounds at the contact with water.*

Studies have been performed on ammonium compounds removal by adsorption on active carbon and ion exchange processes on natural zeolites.

Key Words: water treatment, ammonium, adsorption, ion exchange, oxidation, natural zeolites

Reference:

[1] A.G Tekerlekopoulou,. and D.V Vayenas, 2007, *Desalination*, 210, 225-235.

[2] A.G. Tekerlekopoulou, S. Pavloub, and D. V. Vayenasa, *J Chem Technol Biotechnol* 2013; 88: 751–773

[3] E. Okoniewska, J., Lach, M. Kacprzak,. and E. Neczaj, 2007 *Desalination*, 206, 251-258.

[4] N. Kontari, *Water Eng. Man.*, 1988, 135, 25-26.

[5] S. Edwards, R. Alharthi and A.E. Ghaly, American J. of Environ. Sci., 2011, 7 (4): 295-305.

[6] WSA, Water Security Agency, 2012, http://www.saskh20.ca/DWBinder/epb431.pdf

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BOOK OF ABSTRACTS

SICHEM – 2024

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

1. Keynotes

SB-KN01 A NEW APPROACH BASED ON THE ANALYSIS OF THE COMPLEX CONDUCTIVITY FOR THE IDENTIFICATION OF THE OPTIMUM ENTANGLEMENT CONCENTRATION OF POLYSACCHARIDE IN AQUEOUS SOLUTIONS

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Abstract: *The evolution of the complex conductivity of raw polysaccharide extracted from Cystoseira myriophyloides algae showed strong temperature dependence. Two relaxation processes at medium and high frequency related to the bulk behavior were identified and were described by the Cole-Cole relaxation. The origin of each relaxation is attributed to the electrostatic interactions between the molecular chains and the counter ions which lead to generate Maxwell-Wagner-Sillars (MWS) interfacial polarizations. The relaxation at medium frequency was assigned to a part of the counter ions; which can be found more tightly bounded within more compact structure inside of the surface between the two adjacent molecular due the crosslinking. Whereas the relaxation at high frequency was assigned to the other counter ions; which can be found less bounded outside of the surface between the adjacent molecular.*

Keywords: *Raw polysaccharides, Complex conductivity, Equivalent circuit, Activation energy.*

Introduction: Our recent study has focused on the analysis of the complex impedance and conductivity of polysaccharide concentrations from 2 to 7% (w/v) at room temperature. This study has revealed that all parameters extracted from the relaxation processes exhibited a net transition from dilute to semi-dilute behavior occurring above 5% (w/v). Therefore, the concentration of 7% (w/v) was selected in the semi-dilute behavior for further investigation at different temperatures.

Experimental and/or Modelling: The analysis of the complex conductivity versus frequency was investigated through an appropriate electrical circuit based on our theoretical approach; which allowed to the generation of analytical functions representative of the relaxations process involved at different temperatures. Then; an extrapolation and deconvolution procedure was employed to further investigate this analysis and to identify all relaxation processes and their origin. All these approaches revealed the existence of three relaxation processes: The first one observed at low frequency is attributed to the interfacial polarization between the electrode and the solution. The second and the third observed at medium and high frequency are attributed to the bulk's relaxation processes. In this case, a subtraction

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of the low-frequency process allowed us to make the two for the bulk's relaxation processes more clear for the bulk's relaxation.

Conclusions: The conductivity relaxation processes are found to be thermally activated. The temperature dependence of the useful parameters extracted from each relaxation; such as relaxation time (τ_σ) and (σ_{dc}) as well as (σ_ω) conductivity; exhibited Arrhenius law behavior. Moreover; the activation energy values for each relaxation process were obtained and a linear good correlation between the activation energies values related to the relaxation time (τ_σ) and the (σ_{dc}) and (σ_ω) was also established.

References:

[1] Zaim S.,**Sabir I.**, Rchid H., Ursu A.V., Vial C., Michaud P., Nmila R., El Moznine R. *First derivative, extrapolation, and deconvolution of the complex conductivity data for the identification of the optimum entanglement concentration of polysaccharides in aqueous solutions*. Applied Physics A (2024).

About author

Reddad EL MOZNINE is a full Professor at University Chouaib Doukkali of El Jadida, Morocco. He is the responsible of the Impedance Spectroscopy Research Group at Laboratory of Condensed Matter Physics (LPCM). He focuses in particular on the development of new approaches for a microscopic understanding on their behavior in combination with rheological properties and according to their applications fields. He coordinated many international scientific partnership (PHC Toubkal ...). He is the advisor and co-advisor for 16 PhD students with 10 who already defended their thesis. He has published more than 60 research papers and chapter book and participated on 100 international and national conference proceeding. He worked also on different industrial project as a Research Scientist at Wisconsin Center of Adhesives and Sealant Science, Virginia Polytechnic Institute and State University, USA (1998), at Astra-Zeneca at De Montfort University, Leicester, UK etc. His research interests are centered on the behavior of the dielectric/electric and the rheological properties of materials.

He is a member of scientific associations for Valorization of Natural Resources and Sustainable Development "SMAVARN-2D".

BOOK OF ABSTRACTS

SICHEM – 2024

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

2. Oral presentations

SB-OP01 CIRCULAR ECONOMY BASED SOLUTIONS DEMONSTRATING THE EFFICIENT RECOVERY OF VALUABLE MATERIAL RESOURCES FROM THE CONSTRUCTION AND DEMOLITION WASTE

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Abstract: *The main objective is to develop and demonstrate novel cost-effective circular smart solutions for an upgraded recovery of secondary building raw materials along the entire circular value chain: from End-of-Life Building materials (EBM) to new building products prepared for circularity and resource-efficiency in built environment. The goal was to enhance the development and demonstration of intelligent solutions that improve the cost-effectiveness, reliability, and performance of quantifying, tracing, and managing EBM. The focus was on designing, developing, and demonstrating cost-effective building products designed for easy disassembly and resource efficiency, encompassing both materials and energy. This involved substituting significant portions (30-100 wt%) of virgin raw materials with high-purity recycled building materials.*

Key words: Circular economy, Waste recycling, Environment, resources and sustainability.

Introduction: EU28 generates around 350 Mt [1] of construction, renovation and demolition waste, excluding excavation wastes. As part of a continuous effort towards a sustainable economy, the European Commission adopted in 2015 a new Circular Economy (CE) Package [2] with measures prioritizing EBM among others. The study proposes integral recovery solutions for EBM overcoming the main barriers hindering the CE in buildings throughout the whole building value chain.

Experimental and/or Modelling: In the material development phase, technical performance characteristics ((mechanical, chemical, and durability) of eco-hybrid cement were determined following the EN 196 standard and compared with market-ready alternatives. Structural precast elements made from recycled concrete (comprising over 75% recycled concrete aggregates and Eco-hybrid cement) were designed, manufactured, and tested using scaled-down versions ranging from 1/2 to 1/3 in size.

Results and discussions: The results indicated that EBMs can effectively function as raw materials in construction materials, demonstrating performance similar to their virgin counterparts while meeting relevant standards. Waste materials can be utilized as value-added raw materials in the built environment, enabling the implementation of a circular economy model in construction sector. It has been demonstrated that millions of tons of waste currently occupying landfill sites can be reintegrated into the economy. This not only addresses global pollution issues caused by these wastes but also frees up land space, which can be used for other purposes. Moreover, it provides valuable resources for new construction activities. Utilizing the research findings, the structure presented in Figure 1 was constructed

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using building materials containing EBMs, indicating possibility of utilizing EBM in built environment.

Fig. 1 Precast building constructed using EBM-based construction materials.

Conclusions: This study outputs will drive substantial progress in the adoption of the circular economy within the building industry. This will be achieved through the development of innovative tools for circular reverse logistics and advanced technologies for producing high-value secondary raw materials. These efforts aim to establish market confidence and acceptance of recycled EBM.

References:

[1] Deloitte, 2017, Resource Efficient Use of Mixed Wastes-Improving management of C&DW
[2] EC COM 2015, Closing the loop-A, EU action plan for the Circular Economy

SB-OP02 MULTIVARIATE STATISTICAL TOOLS FOR APICULTURAL PRODUCS QALITY EVALUATION BASED ON SPECTRAL INFORMATION

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Abstract: *UV-Vis spectral data were treated using multivariate statistical methods to evaluate the quality of Romanian honey. The present study demonstrates that UV-Vis spectral data may be used to identify significant differences between genuine honey and adulterated ones by using adequate multivariate statistical tools in treating the information. Partial Component Analysis (PCA) and Linear Discriminant Analysis (LDA) were used in the classification of spectral data. Partial Least Squares (PLS) corelated the degree of adulteration of each honey type with the spectral data.*

Key words: UV-Vis spectra, honey adulteration identification, PCA, LDA, PLS

Introduction: Although the number of consumers of honey has increased in recent years, their trust and interest in this valuable product has decreased as often adulterated honey can be found on the market. The necessity of honey adulteration identification is obvious and rapid, reliable, and affordable instruments are necessary [1,2]. UV-Vis spectra prove to be useful in such an attempt [3], while allowing a rapid estimation of other qualities of an apicultural product, such as the antioxidant capacity.

Experimental and/or Modelling: UV-Vis spectra were recorded for 6 genuine hones of different types, 5 commonly used syrups on the Romanian market, and 84 directly adulterated honeys samples (adulterant concentration varied in the 5% - 50% range). The 220-380 nm spectral data were used for classification by PCA and LDA. The antioxidant capacity of some adulterated honey samples measured by the DPPH method were correlated with the spectral information using PLS.

Results and discussions: PCA applied to the UV-Vis spectral data (Figure 1) put into evidence a sample grouping, more evident after applying LDA using the first 10 PCs (figure 2). Some test samples were used to validate the capacity of LDA method to identify new adulterated honeys. The test samples were correctly assigned to the adulterated honey groups in the LDA coordinates. Based on these results a large data base can be built up and used in future attempts to evaluate the quality of honey on the Romanian Market. A partial least squares regression was applied to correlate the spectral data of pure honey and adulterated ones with the rage of adulteration (between 0.05 and 0.5 mass fractions). Some test samples were used to validate the correlation.

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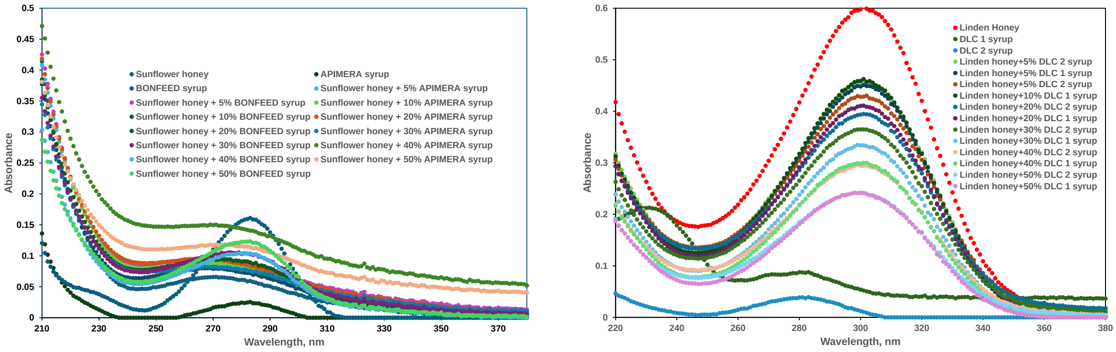

a) **b)**

Figure 1. Spectral information for monitoring the direct adulteration of sunflower (a) and linden (b) honey with APIMERA, BONFFED, and DLC 1 and DLC 2 plant syrups.

Figure 3 presents the results obtained for sunflower honeys adulterated with glucose syrup.

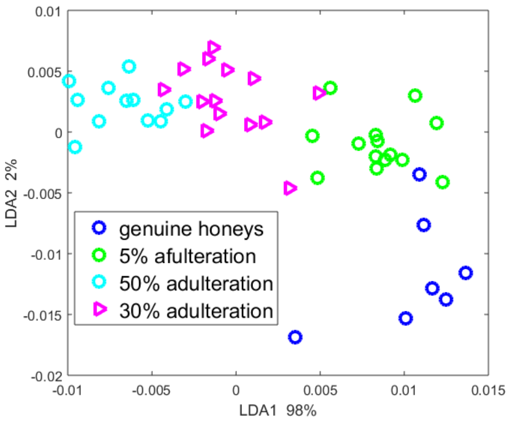

Figure 2 Representation of the analyzed samples in LDA directions

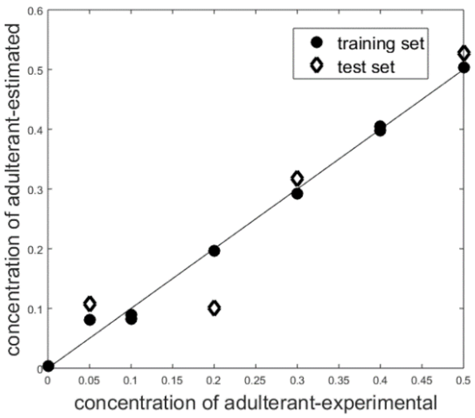

Figure 3. Parity plot for the correlation of the degree of adulteration of sunflower honeys

Conclusions: Statistical tools proved to be adequate in classifying genuine and adulterated honeys and estimating the degree of adulteration using UV-Vis spectra.

References:

[1] Benkovic, M., Jurina, T., Longin, L., Grbeš, F., Valinger, D., Jurinjak Tušek, A., Gajdoš Kljusuric J. Qualitative and Quantitative Detection of Acacia Honey Adulteration with Glucose Syrup using Near-Infrared Spectroscopy. *Separations* 9 (2022), 312. https://doi.org/10.3390/separations9100312.

[2] Pauliuc, D.; Ciursa, P.; Ropciuc, S.; Dranca, F.; Oroian, M. Physicochemical parameters prediction and authentication of different monofloral honeys based on FTIR spectra. *J. Food Compos. Anal*. 102 (2021), 104021, https://doi.org/10.1016/j.jfca.2021.104021

[3] Nunes, A., Lima, P., Azevedo, G. Z., Moura, S., Rocha dos Santos, B., Maraschin, M. Application of UV–vis spectrophotometry and chemometrics to investigate adulteration by glucose syrup in Brazilian polyfloral honey. *Food and Humanity*, 2 (2024), 100194, https://doi.org/10.1016/j.foohum.2023.12.002.

SB-OP03 BIODEGRADABLE CHITOSAN/QUATERNIZED CHITOSAN NANOFIBERS LINKED WITH AN ANTIOXIDANT COMPOUND FOR THE DELIVERY OF ERYTHROMYCIN

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***Abstract**: Formulating drugs as nanofibers for topical application offers advantages, particularly with erythromycin (ERY). Chitosan (CS), known for its biocompatibility and antimicrobial properties, was used to embed ERY into nanofibers with quaternized chitosan (HTCC). The resulting composite, bonded with an active compound through imine linkage, showed promising results in in vivo studies.*

Key words: Drug-delivery, Biomaterials, Nanofibers

Introduction: Erythromycin, a widely-used antibiotic renowned for its efficacy against various bacterial infections, presents distinctive advantages when formulated as nanofibers for topical applications. [1]. This study aims to elucidate the benefits of employing erythromycin-loaded imino-linked chitosan nanofibers, with a specific focus on the evaluation of their biological properties, thereby enhancing therapeutic outcomes in dermatological and wound healing treatments.

Experimental and/or Modelling: *Materials:* CS, ERY, HTCC, 2-hydroxy-5-methoxybenzaldehyde (2H5M), polyethylene oxide (PEO)*; Preparation:* electrospinning, drug loading and imination*; Evaluation of fibers activity in aqueous solutions:* swelling behaviour, release studies, biodegradation studies, bioadhesive properties*; Evaluation of properties for the desired application:* antioxidant activity, quantification and release kinetics of the active compounds, antimicrobial activity and *in vivo* biocompatibility.

Results and discussions: A series of chitosan-based nanofibers were prepared, incorporating two distinct agents: the antibiotic erythromycin (ERY) and a natural aldehyde (2H5M). [2]. These agents were loaded separately or in combination within the fibers. The nanofibers were obtained by needleless electrospinning technique followed by PEO removal, loading with ERY and/or reacting at the surface with 2H5M (Fig. 1). The structural and morphological characterization showed an effective drug loading and imination reaction, as well as a succesful removal of PEO. The investigations revealed an improvement in ERY release kinetics following imination, promising antioxidant capacity, good antimicrobial activity over a broad-spectrum of pathogens and good biocompatibility on rats.

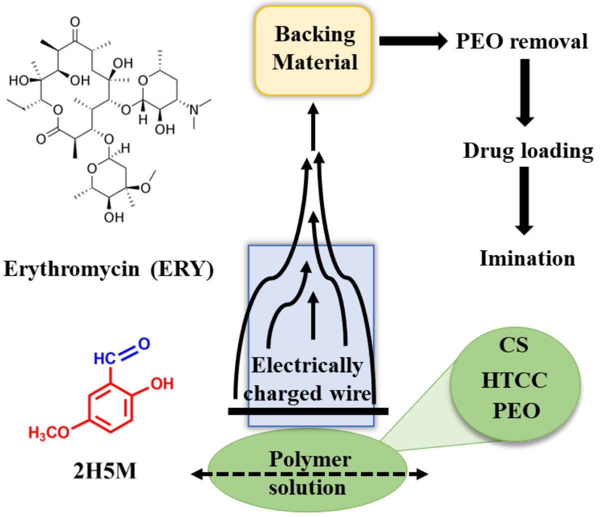

Fig. 1 General preparation scheme of the formulation.

Conclusions: The obtained fibers revealed both a good antioxidant capacity, as well as antimicrobial activity, making them suitable for biomedical applications.

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References:

[1] Doostan, M., Maleki, H., Doostan, M., Khoshnevisan, K., Faridi-Majidi, R. and Arkan, E., 2021. Effective antibacterial electrospun cellulose acetate nanofibrous patches containing chitosan/erythromycin nanoparticles. *International journal of biological macromolecules*, *168*, pp.464-473.

[2] Kundu, A. and Mitra, A., 2016. Methoxybenzaldehydes in plants: insight to the natural resources, isolation, application and biosynthesis. *Current science*, pp.1325-1334.

SB-OP04 THE INFLUENCE OF MASS TRANSPORT ON THE ELECTROCRYSTALLISATION PROCESS

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Abstract: *Electrocrystallisation is an essential elemental process used for deposition of metals from aqueous electrolytes. In an electrolyte solution, ion-solvent interactions and ion-ion interactions can take place, the predominant ones being of the ion-ion type. The mass transport of ions through the electrolyte can limit the rate of the electrode process based on reduction of metal ions. The speed of this elementary process depends on the value of current density and becomes significant if the electrolyte is operated at relatively high current densities. The higher the electrode polarizations for the elementary electrocrystallization process, the better the quality of the cathodic deposits can be.*

Key words: cooper, electrode overpotential, electrolytes electroplating.

Introduction: Mass transport can limit the speed of electrode processes, its rate depends on the current density value of the electrolyte. In the case of slow electrochemical reactions that take place at low and very low current densities, the concentration difference between the bulk of the electrolyte and the immediate vicinity of the electrode-electrolyte interface is small, resulting in mass transport not being the determining factor for reaction rate. Fast electrochemical reactions, carried out at high current densities, can be limited by the rate of mass transport to the electrode [1-4]. The electrode overpotential corresponding to mass transport, expressed through the limiting current density, can be calculated using the following formula:

$$\eta_d = -\frac{R \cdot T}{z_i \cdot F} \cdot ln\left(1 - \frac{i}{i_d}\right) \text{, [V]}$$

Modelling: To establish the current passing through the reactor, expressions are written that give the current density as a function of the ionic flux to the two electrodes:

$$i_+ = z_+ F \cdot \left(N_+\right)_{x=0} \qquad \text{and} \qquad i_- = z_- F \cdot \left(N_-\right)_{x=d}$$

The transport number of cations, and respectively the transport number of anions can be written as:

$$\frac{i_+}{i} = \frac{z_+ \cdot N_+^v}{z_+ \cdot N_+^v + z_- \cdot N_-^v} = t_+ \qquad \text{and} \qquad \frac{i_-}{i} = \frac{z_- \cdot N_-^v}{z_+ \cdot N_+^v + z_- \cdot N_-^v} = t_-$$

The transport numbers of the ions will be equal to:

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$$t_+ = \frac{z_+ \cdot D_+^v}{z_- \cdot D_-^v \; - \; z_+ \cdot D_+^v} \qquad \text{and} \qquad t_- = \frac{z_- \cdot D_-^v}{z_- \cdot D_-^v \; - \; z_+ \cdot D_+^v}$$

The cathodic current density during the electrolysis of a binary electrolyte solution is expressed through the expression:

$$\frac{i}{z_+ F} = -\frac{D_{exp}}{1-\left(t_+\right)_{x=0}} \cdot \left(\frac{dC_+}{dx}\right)_{x=0}$$

Results and discussions: The verification of the mass transport influence on the electrochemical process parameters was carried out in the case of electrochemical deposition of copper using two types of electrolytes [5]: (a) *cyanuric electrolytes*, for which the current density is less than 10 A/dm^2, are characterized by exceptional penetrating power, the deposits having a fine structure, special adhesion, and uniform thickness; (b) *sulphate electrolytes*, for which the current density is higher than 100 A/dm^2 even reaching 1500 A/dm^2; these electrolytes are characterized by high chemical stability, high current efficiencies, but with relatively low penetrating power, with deposits exhibiting a coarse structure. The calculations of the transfer overpotential for cyanuric electrolytes and sulphate electrolytes characteristic for copper electrodeposition was performed for the range of i/i_d = 0,7 – 0,99 and temperature range between 18 – 25 ^{0}C.

Conclusions: Quality galvanic deposits are formed by numerous, fine crystals, which give the resulting layer adhesion, porosity as low as possible, hardness and a thickness as uniform as possible. The speed of formation of solid phase nuclei is much higher than their growth rate [2, 4, 6]. The higher the electrode polarizations in deposits from a particular electrolyte, the better the quality of the cathodic deposits can be. The electrodeposition of Cu^+, for cyanide electrolytes, the mass transfer overpotential value is twice as large as that corresponding to the deposition of Cu^{2+} from acidic electrolytes. The high values of mass transfer overpotential that occur in the case of cyanide electrolytes ensure the formation of quality deposits. For this reason, cyanide electrolytes are preferred over acidic ones, even though it requires a technological step for wastewater treatment.

References:

[1] Oniciu L., Constantinecu C., *Electrochimie şi coroziune*, Editura Didactică şi Pedagogică, Bucureşti, 1982.

[2] Scott K., *Electrochemical Reaction Engineering*, Academic Press, Londra, 1991.

[3] Okagaki J., Hsu W.L., Chisaka M., Yoo E., Matsuda H., Daiguji H., Simple method of determining the ion transport parameters of binary liquid electrolytes, *Journal of Electroanalytical Chemistry*, 929, (2023), 117105.

[4] Low C.T.J., Ponce de Leon C., Walsh F.C., Electrodeposition of copper from mixed sulphate–chloride acidic electrolytes at a rotating disc electrode, *The International Journal of Surface Engineering and Coatings*, 92, (2014), 281-288.

[5] Firoiu C., *Tehnologia proceselor electrochimice*, Editura Didactică şi Pedagogică, Bucureşti, 1983.

[6] Choo R.T.C., Toguri J.M., El-Sherik A.M., Erb U., Mass transfer and electrocrystallization analyses of nanocrystalline nickel production by pulse plating, *Journal of Applied Electrochemistry*, 25, (1995), 384-403.

SB-OP05 INFLUENCE OF FLUORINE LATERAL SUBSTITUTION ON PHOTOISOMERIZATION PROCESS OF AZOBENZENE BENT-CORE LIQUID CRYSTALS

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Abstract: *This study concerns the photoisomerization process and thermal back relaxation of fluorine substituted azobenzene bent-core liquid crystals. The studied bent-core compounds are resorcinol derivatives with a symmetric molecule, incorporated photosensitive azo linkages in the fluorine-substituted side arms and alkoxy terminal chains. The effect of polar fluorine substituents on the azobenzene side arms of bent core molecules on the photoisomerization process was investigated using UV-Vis spectroscopy. It has been shown that the trans-cis isomerization process by 400 nm UV irradiation is not affected by fluorine substitution. While the thermal back relaxation process is considerably influenced, therefore the thermal relaxation time increased proportionally with the number of side fluorine substituents. Taking into account that thermal relaxation time is of crucial importance for optical storage devices, lateral substitution with fluorine atoms is an efficient method to obtain bent-core photosensitive materials with long thermal back relaxation time.*

Key words: bent-core liquid crystals, azobenzene linkage, photoisomerization, fluorine substitution, optical storage devices. (TNR 10)

Introduction: In the field of liquid crystal research, photosensitive bent-core compounds have recently attracted attention [1,2]. Due to the unique properties of the photosensitive azobenzene units. They can switch from trans to cis isomer by irradiation with UV light and reverse by thermal back relaxation [3,4]. These properties lead to a variety of applications such as, optical storage devices[5], photo iduced phase transition[6] or optical switching[7]. This paper presents the study of photoisomerization and thermal back relaxation process of fluoro substetuted bent-core compounds. (TNR 12, 1R , 5-6 lines)

Experimental: A Varian Cary 3500 UV-Vis spectrophotometer connected with a small Peltier apparatus was used to perform UV spectroscopy investigations in chloroform solutions at 10^{-5} mol/L using 10 mm pathlength quartz cuvettes with Teflon stoppers. For the irradiation, two commercial LEDs from Thorlabs, the "M455L2-C4" model with a wavelength of 455 nm and a commercial "Varta" lamp with a maximum wavelength of 400 nm were chosen.

Results and discussions: The synthesis and mesomorphic characterization of bent-core compounds used in this study was reported earlier [8]. Figure 1a) shows that,

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prior to irradiation, the bent-core compound was in the energetically favorable trans conformation. Twenty seconds after being exposed to 400 nm wavelength UV light, compound NC12 switch to the cis configuration. The reverse process can be performed in two ways, irradiation with visible light Figure 1. b), which requires 20 sec of irradiation or thermal back relaxation in 70 min at 45 °C for the unsubstituted compound (NC12). In the case of fluorine-substituted compounds, the trans-cis isomerization process takes the same amount of time to complete, but the thermal relaxation process takes significantly longer—130 minutes for compounds containing two fluorine atoms and 220 minutes for compounds containing four fluorine atoms.

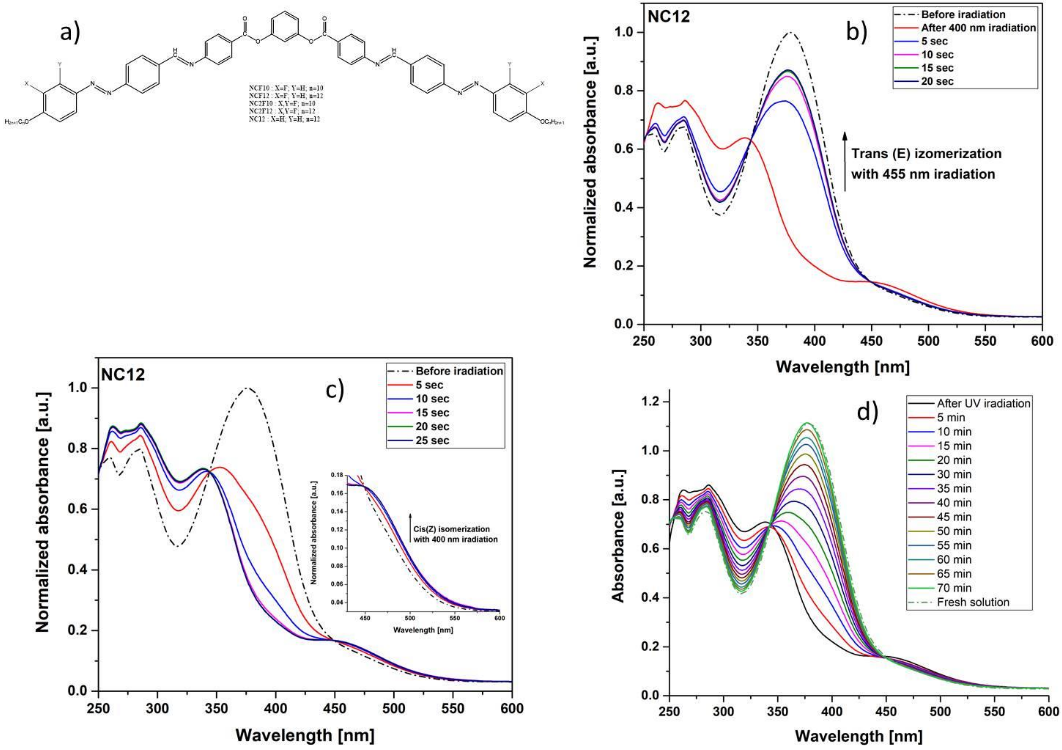

Fig. 1. Molecular structure and absorbance bands of compound NC12: a) molecular structure of bent-core azobenzene compound; b) cis-trans isomerization with visible blue light; c) trans-cis isomerization with 400 nm UV light; d) thermal back relaxation at 45 °C.

Conclusions: In conclusion, bent-core azobenzene compounds are photoisomerisable; this process can be done in 20 seconds by irradiation with UV or visible light. The back thermal relaxation process is influenced by the lateral substitution of fluorine atoms and lasts from 70 to 220 min, depending on the number of substituents.

References:

[1] Srinivasan, M. V., Kannan, P. & Roy, A. Photo and electrically switchable B-7 mesophase exhibiting asymmetric bent-core liquid crystals. *New J. Chem.* 37, (2013), 1584-1590.

[2] Cigl, M. et al. Photosensitive chiral self-assembling materials: significant effects of small lateral substituents. *J. Mater. Chem. C*, 4, (2016), 5326-5333.

[3] Ting, T. X., Sarjadi, M. S. & Rahman, M. L. Influences of Central Units and Terminal Chains on the Banana-Shaped Liquid Crystals. *Crystals* 10, (2020), 857.

[4] Vijaysrinivasan, M., Kannan, P. & Roy, A. Dual switchable six-ring bent-core liquid crystals with azo linkages exhibiting B-1 and B-2 mesophases. *Liq. Cryst.* 39, (2012), 1465–1475.

[5] Sunil, B. N. et al. Effective tuning of optical storage devices using photosensitive bent-core liquid crystals. *J. Mol. Liq.* 304, (2020), 112719.

[6] Prasad, S. K., Nair, G. G. & Rao, D. S. S. Photoinduced phase transitions. *Liq. Cryst.* 36, (2009), 705–716.

[7] Saravanan, C., Senthil, S. & Kannan, P. Click chemistry-assisted triazole-substituted azobenzene and fulgimide units in the pendant-based copoly(decyloxymethacrylate)s for dual-mode optical switches. *J. Polym. Sci. Part Polym. Chem.* 46, (2008), 7843–7860.

[8] Berladean, I. et al. Novel antiferroelectric materials with resorcinol-based symmetrical fluorinated bent-core mesogens. *J. Mol. Liq.* 388, (2023), 122753.

SB-OP06 SIMULTANEOUS REMOVAL OF NITRATE AND SULFATE FROM GROUNDWATER BY BATCH ELECTROCOAGULATION PROCESS USING IRON ELECTRODES

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Abstract: *Electrocoagulation using iron electrodes was proposed as an alternative method for the simultaneous removal of nitrate and sulfate ions from groundwater. The effect of the initial ratio between sulfate and nitrate concentration ($[SO_4^{2-}]/[NO_3^-]$) on the performance of the process was evaluated. The main mechanism involved in nitrate and sulfate removal by EC was also investigated.*

Key words: Electrocoagulation, iron electrodes, nitrate, sulfate, groundwater, ratio $[SO_4^{2-}]/[NO_3^-]$

Introduction: Nitrate and sulfate ions were identified as the most common groundwater contaminants worldwide. The infiltration of chemical fertilizers, mineral dissolution and mining operation were reported as the main sources of groundwater contamination by nitrate and sulfate [1, 2]. Once used for human consumption, high levels of nitrate and sulfate in groundwater, exceeding the WHO recommendations of 50 mg NO_3^- L^{-1} and 250 mg SO_4^{2-} L^{-1} [3] may cause hazardous diseases in humans [1, 2]. The aim of this work was to apply electrocoagulation (EC) in batch mode to remove nitrate and sulfate ions from groundwater in order to provide safe drinking water.

Experimental: The experimental setup consisted in a batch electrochemical cell containing 500 mL of several synthetic groundwater (GW) samples contaminated with 148 mg NO_3^- L^{-1} and different concentrations of SO_4^{2-} in the following mass ratios R ($[SO_4^{2-}]/[NO_3^-]$): 0.5, 1.0, 2.0, and 4.0. Two iron electrodes, with 42 cm^2 of immersed area, served to conduct electric current at a current density of 42.8 mA cm^{-2} during 120 min. Ion chromatography (Metrohm AG, 882 Compact IC plus, Switzerland) was used to assess nitrate, nitrogen by-products, and sulfate concentrations. Total nitrogen (TN) in both liquid and solid phases was measured using a total nitrogen analyzer (TNM-1, Shimadzu, Japan).

Results and discussions: As illustrated in figure 1, $[NO_3^-]$ and $[SO_4^{2-}]$ were shown to decrease during 120 min of EC. Regardless of R, $[NO_3^-]$ decreased under the WHO recommendation. For the sulfate-free water, the nitrate removal yield was

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about 99.8 %. Conversely, it was observed that denitrification yield slightly decreased for groundwater samples with R > 1.0, it went from 97.2 to 94.2, and to 88.1 % when R increased from 0.5 to 2.0, and to 4.0, respectively. Thus, it was highlighted that nitrate removal could be significantly influenced by [SO_4^{2-}] at R > 2.0. IC and TN analysis showed that nitrate ions were mainly reduced into ammonium cations and nitrogen gas at the iron cathode. At R > 2.0, sulfate ions may decrease the contact of nitrate with the cathode, which decreased the denitrification yield. Similarly, it was observed that sulfate removal yield decreased when increasing R, it went from 64.7 to 27.9 % when R increased from 0.5 to 4.0. At R=4.0, [SO_4^{2-}] remained above the WHO recommendation. At fixed [NO_3^-], the increase in [SO_4^{2-}] may decrease the sulfate removal as more sulfate ions are present in groundwater and the fixed amount of iron flocs formed after anode dissolution cannot adsorb all available sulfate ions. Actually, the amount of sulfates removed by EC increased when R increased from 0,5 to 4.0 despite the decrease in removal yield.

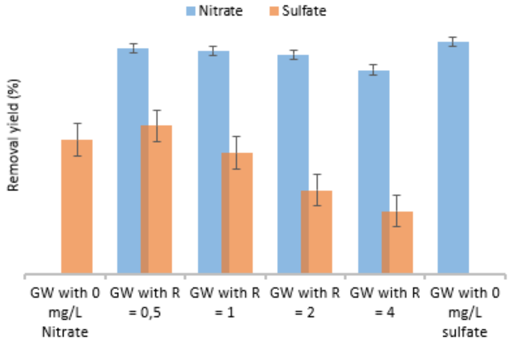

Fig. 1 Nitrate and sulfate removal yields after 120 min of EC

Conclusion: This study allowed us to prove the feasibility of EC as an alternative to classical methods for the simultaneous removal of nitrate and sulfate from groundwater. It can be concluded that the efficiency of the process strongly depends on the [SO_4^{2-}]/[NO_3^-] ratio, which must not exceed 2. The results from this work will be used in the study of groundwater treatment by EC in continuous mode.

References:

[1] Athina Ziouvelou, Athanasia G. Tekerlekopoulou, Dimitris V. Vayenas, A hybrid system for groundwater denitrification using electrocoagulation and adsorption, Journal of Environmental Management, 249, (2019), 109355.

[2] Matteo Tucci, Cruz Viggi Carolina, Marco Resitano, Bruna Matturro, Simona Crognale, Ilaria Pietrini, Simona Rossetti, Falk Harnisch, Federico Aulenta, Simultaneous removal of hydrocarbons and sulfate from groundwater using a "bioelectric well", Electrochimica Acta, 388, (2021), 138636.

[3] Guidelines for drinking-water quality: *4th ed. incorporating first addendum*. Genève: WHO, 2017. License: CC BY-NC-SA 3.0 IGO.

SB-OP07 ADVANCING IMMOBILIZED ENZYME REACTOR SYSTEMS FOR VERSITILE EXPLOITATION OF FUNCTIONAL POLYSACCHARIDES AND ACTIVE OLIGOSACCHARIDES

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Abstract:* The exploitation of functional polysaccharides and active oligosaccharides has attracted extensive interest due to their applications in the fields of cosmetics, health, nutraceuticals, food, etc. During the last decade, immobilized enzymatic catalysis as a green-chemistry method has been used to make polysaccharide molecular modifications and develop new active oligosaccharides. In this research, an immobilized enzyme reactor system was built, composed of two main enzymatic compartments. The first compartment aims to add phenol groups onto polysaccharides, consisting of a monolithic Convective Interaction Media® carboxy imidazole (CIM® CDI) disk with immobilized laccases (EC 1.10.3.2) from Trametes versicolor. Dextran T40, used as a model polysaccharide, was employed to assess the process. The second compartment was used to deconstruct polysaccharides, thus producing oligosaccharides. Glucuronan lyases (EC 4.2.2.14) from Rhizobium rosettiformans were immobilized on a CIM® CDI disk to deconstruct glucuronan. In both compartments, the kinetic parameters of free and immobilized enzymes were quantified, including the maximum rate (V_{max}) and Michaelis constant (K_m). The design of experiments (DOE) and respond surface methodology (RSM) were used to explore the operating effects on enzymatic catalysis for finally optimizing the operating conditions, i.e., substrate concentration, flow rate, and reaction time. The stability of each immobilized enzymes reactor was monitored to evaluate its life span. Finally, we aim to combine these two compartments with a membrane filtration system to build a multistep enzymatic reactor system for polysaccharides and oligosaccharides development.

Key words: Immobilized enzyme reactor, functional polysaccharides, oligosaccharides

Introduction: Enzymatic catalysis, especially immobilized enzymes reactors, is a critical method for exploiting functional polysaccharides and oligosaccharides [1-3]. In this research, laccases and glucuronan lyases were respectively immobilized on CIM® CDI disks to produce functional poly- and oligosaccharides. Immobilization yields, kinetic parameters, operational conditions, and stability of the immobilized enzymes were investigated.

Experimental and/or Modelling: *Reagents:* Convective Interactive Media® (CIM®) carboxy imidazole (CDI) disk, laccases (EC 1.10.3.2) from *Trametes versicolor*, dextran T40, gallic acid, glucuronan lyases (EC 4.2.2.14) from *Rhizobium rosettiformans,* glucuronan; *Immobilization yields:* Bradford method or Lowry method, using bovine serum albumin as standard; *Evaluation of enzymes:*

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phenolization of dextran T40 (laccase), monitoring the depolymerization of glucuronan (glucuronan lyase).

Results and discussions: The immobilization yields for laccases and glucuronan lyases were 32.17% and 63.61% respectively. The maximum rates (V_{max}) and Michaelis constants (K_m) of free and immobilized laccases were 0.0049 and 0.1770 $\mu mol \cdot min^{-1}$, 0.00121 and 0.7510 $mmol \cdot l^{-1}$. For free and immobilized glucuronan lyases, V_{max} and K_m values were 56.216 and 56.863 $\mu M \cdot min^{-1}$, 0.310 and 0.122 $g \cdot l^{-1}$. The response surface results indicated that substrate concentration and reaction time significantly affect the catalysis. The operational stability of immobilized laccases was 91.29%, retaining activity retained after running 1,200 column volumes of substrate. For immobilized glucuronan lyases, this value was closed to 50.9% after running 2,373 column volumes. It's noteworthy that phenolized dextran T40 exhibited antioxidant activity whereas immobilized glucuronan lyases overcame the inhibition observed with free enzymes under high concentrations of glucuronan.

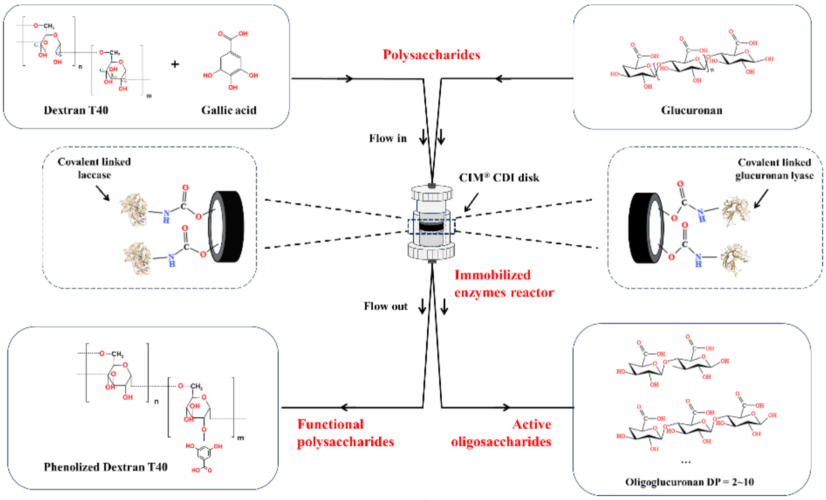

Fig. 1 Schematic diagram of monolithic CIM® CDI reactors immobilized with laccases or glucuronan lyases for producing functional polysaccharides or active oligosaccharides.

Conclusions: Two immobilized enzymes reactors were developed, then a membrane filtration system will be used for oligosaccharides purification in following work.

References:

[1] Li, S., Xiong, Q., Lai, X., et al. Molecular modification of polysaccharides and resulting bioactivities. *Compr. Rev. Food Sci. Food Saf.*, 15, 2, (2016), 237-250.

[2] Belorkar, S. A., Gupta, A. K. Oligosaccharides: a boon from nature's desk. Amb Express, 6, (2016), 1-11.

[3] Su, Z., Luo, J., Li, X., et al. Enzyme membrane reactors for production of oligosaccharides: A review on the interdependence between enzyme reaction and membrane separation. *Sep. Purif. Technol.*, 243, (2020), 116840.

SB-OP08 DEVELOPMENT OF AN ELECTROCHEMICAL METHOD FOR THE MEASUREMENT OF OXIDASES ACTIVITY: APPLICATION TO LACCASES

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Abstract: *Laccases (EC 1.10.3.2) are multi-copper oxidoreductases that catalyse the one-electron oxidation of a wide range of substrates by the concomitant reduction of O_2 to water. This enzyme has great potential to replace chemical catalysis in many fields, such as pulp and paper industry, biorefineries, textile, food, and pharmaceutical industries. Many challenges yet remain to overcome before considering their use at industrial scale. The first barrier is the difficulty to measure their activity and kinetics on complex molecules that are not model substrates. A method of chronopotentiometry coupled with voltammetry has been developed, associated with a knowledge model combining the Nernst and Michaelis-Menten equations, to determine and better understand laccase activity. A model laccase substrate, 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS), was used to develop, test and compare the method to a classical spectrophotometric assay. A laccase from Trametes versicolor was thus assayed and its kinetics parameters determined. A* $V_{max} = 16$ *µmol.L.min*$^{-1}$ *and Km = 68 µM were found using the electrochemical method. These values are very close to those obtained with the classical spectrophotometric assay where* $V_{max} = 15$ *µmol.L.min*$^{-1}$ *and Km = 65 µM.*

Key words: Chronopotentiometry, voltammetry, laccases, enzymatic activity.

Introduction: Laccases represent an interesting and promising enzyme for a wide range of industrial applications as they have a large variety of substrates, from phenols to aromatic amines and lignin-related compounds. However, laccases utilization is hindered by the complexity of their activity measurement as no universal method are available to quantify their action on complex substrates. Here, an electrochemical method was developed to address this issue.

Experimental: *Reagents:* 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) was chosen as the model substrate. A laccase from *Trametes versicolor* was used for the experiments. *Electrochemical assay:* Chronopotentiometric and voltammetric experiments were performed in a cryostat glass cell at 25°C using a Solartron SI 1287 potentiostat/galvanostat with three electrodes: two platinum electrodes as working and counter-electrode and a saturated calomel electrode (SCE) as reference electrode.

Results and discussions: The electrochemical method combined with the Nernst-Michaelis model enabled to determine the kinetic parameters of a laccase from *Trametes versicolor*. The resulting curve is shown **Fig. 1**. Using the chronopotentiometric method associated with cyclic voltammetry, a V_{max} of 16

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µmol.L.min^{-1} and a Km of 68 µM were found, which is very close to the values of 15 µmol.L.min^{-1} and 65 µM for V_{max} and Km respectively, found by the classical spectrophotometric method.

Chronopotentiometry has made it possible to link the evolution over time of the redox potential of the solution to the enzyme kinetics parameters of laccase. Cyclic voltammetry wads used as an additional tool for determining electrochemical parameters used in the Nernst model.

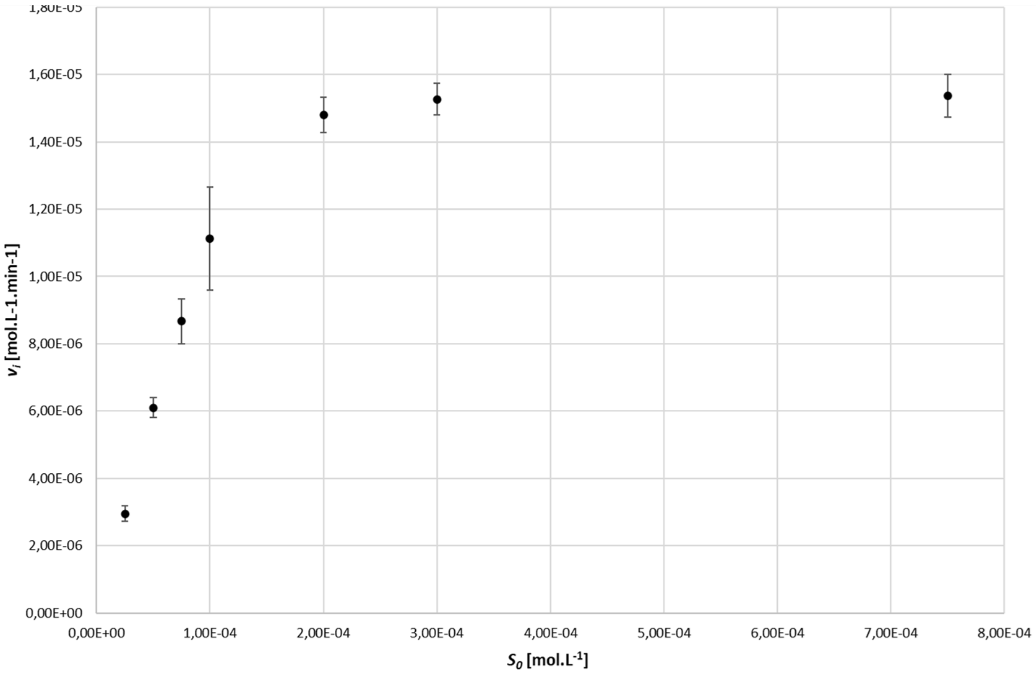

Fig. 1. Michaelis-Menten curve of initial velocity of a laccase from *Trametes versicolor* on ABTS built thanks to an electrochemical method using chronopotentiometry and voltammetry

Conclusion: This study validates the feasibility of using chronopotentiometry to assess the kinetic parameters of laccases on a model substrate, and to explain the theoretical underspinnings of such a method.

SB-OP09 CURRENT RESEARCHES FOR ORGANIC COMPOUNDS REMOVAL USING $BiFeO_3$

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Abstract: *An overview of the synthesis, characteristics and potential applications of $BiFeO_3$ perovskite materials is provided in this communication. The enhanced photocatalytic activity of $BiFeO_3$ compound synthesized via sol-gel method (SG-$BiFeO_3$), for phenol degradation in direct sunlight is preferred versus the co-precipitation, hydrothermal methods. Its advantageous characteristics, such as a reduced energy band gap and effective charge carrier separation, are responsible for SG-$BiFeO_3$'s improved performance. The SG-$BiFeO_3$ sample also shows good stability and recyclability, which makes it a viable option for environmental applications. These results advance our knowledge of $BiFeO_3$-based photocatalysts and their mechanisms of pollutant degradation.*

Key words: Photocatalysis, $BiFeO_3$, pollutant degradation, perovskites, synthesis methods.

Introduction: With its excellent crystal structure properties and visible light photocatalytic activity, easily adjustable structural morphology, bismuth ferrite ($BiFeO_3$) has been shown to exhibit remarkable potential for photocatalytic degradation of water pollutants. Photocatalytic technology has emerged as a promising approach for environmental remediation.**[1]**

Experimental: Three processes are used to produce $BiFeO_3$ nanoparticles: sol-gel, hydrothermal, and co-precipitation. The crystal structure and phase purity of the produced materials are ascertained using XRD examination. To investigate the morphological characteristics and particle size distribution, SEM imaging is used. By observing how organic contaminants degrade in the presence of visible light, the photocatalytic activity of the $BiFeO_3$ samples is assessed.

Results and discussions: In this field, $BiFeO_3$ (BFO) is a well-known material. With a tiny bandgap of 2.1 eV, it is a single-phase semiconductor with outstanding chemical stability. Chang et al. conducted a study on the use of BFO for the photocatalytic degradation of phenol, Fig. 1. The researchers generated sheet-like, coral-like, and rod-like structures by hydrothermal, sol–gel, and coprecipitation synthesis techniques, respectively. The sample made with the sol-gel technique showed improved phenol degradation (98.9%) in 120 minutes under direct sunlight. The removal efficiencies of the BFO samples produced by hydrothermal and coprecipitation techniques were 77.4% and 66.9%, respectively [2].

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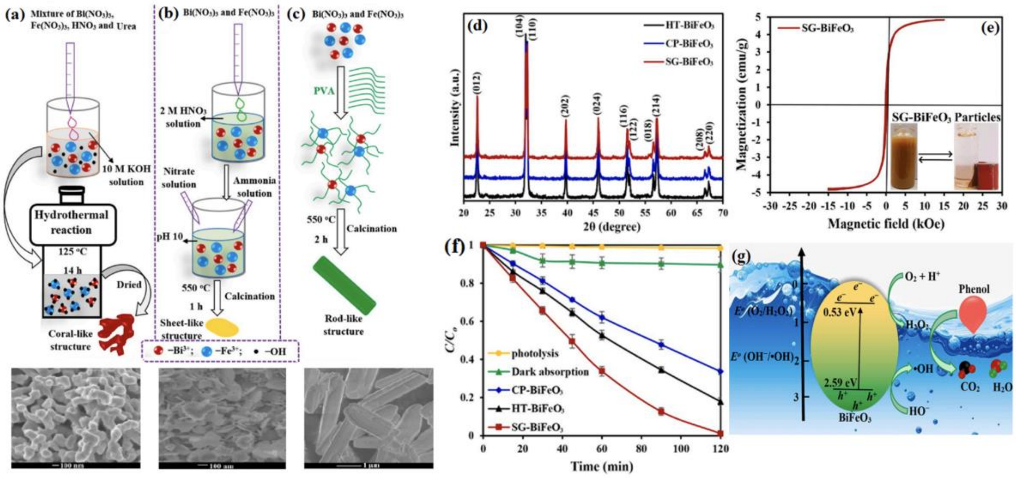

Fig. 1 $BiFeO_3$ (BFO) synthesis via the (a) hydrothermal route, (b) coprecipitation method, (c) sol–gel technique (d) X-ray diffraction patterns of the BFO samples, (e) M–H loop of the sol–gel BFO, (f) photocatalytic degradation of phenol via photolysis, and (g) a proposed schematic diagram for the photodegradation process. Adapted from [2]

Conclusions: The sol-gel synthesis approach is the best option for obtaining of $BiFeO_3$ photocatalysts, that are specifically designed to remove organic contaminants from water.

References:

[1] Zhou T., *et al.*, Strategies for enhancing performance of perovskite bismuth ferrite photocatalysts ($BiFeO_3$): A comprehensive review, *Chemosphere*, 339, (2023), 139678.

[2] Chang Chien S.W., Ng D. Q, Kumar D., Lam S.M., Jaffari Z. H., Investigating the effects of various synthesis routes on morphological, optical, photoelectrochemical and photocatalytic properties of single-phase perovskite BiFeO3, *J. Phys. Chem. Solids*, 160, (2022), 110342.

SB-OP10 METHODS FOR ANTIBIOTICS REMOVAL: A COMPREHENSIVE ANALYSIS

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Abstract: *Antibiotics are essential pharmaceuticals utilized globally for the treatment of bacterial infections. However, their widespread use has led to the presence of antibiotic residues in water bodies, posing environmental and health concerns. This article provides an overview of various classes of antibiotics and their impact on water quality. Furthermore, it explores the effectiveness of three primary removal methods: adsorption, advanced oxidation, and electrochemical processes. Advantages and disadvantages of each method are discussed, considering factors such as efficiency, cost-effectiveness, and environmental impact. Understanding the complexities and trade-offs associated with these removal techniques is crucial for the development of sustainable water treatment strategies aimed at mitigating antibiotic contamination in aquatic ecosystems.*

Key words: adsorption, antibiotics, fenton, oxidation

Introduction: The toxic effects of antibiotics in water include treatment failure, prolonging the duration of illnesses, and increasing mortality rates, which are causing high human and economic costs to society. According to the chemical structure can be seen in fig 1, they are divided into different classes (Phoon et al., 2020)

Fig. 1 Antibiotics classification.

Experimental methods of antibiotics removal from wastewater:

Currently, numerous experimental methods exist for removing antibiotics from wastewater, including chemical methods, physical methods, advanced oxidation and biological methods.

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Results and discussions: In recent years, there has been significant progress in the removal of medicinal substances from water, driven by experimental advancements. This development is particularly crucial due to the rising concentrations of antibiotics in water sources.

Additionally, understanding the correlation between the chemical structure of antibiotics and the physico-chemical removal methods employed is essential for effective characterization.

Throughout the process of adsorbing pharmaceutical substances, the interactions between the adsorbent and the active compound encompass a variety of bonding mechanisms, such as physical bonds, weak chemical bonds, electrostatic interactions or donor-acceptor interactions.

AOPs are classified into two categories: non-photochemical AOPs (such as ozonation, Fenton, and electrolysis) and photochemical AOPs (such as photolysis, photocatalysis, and photo-Fenton).

The electrochemical oxidation process involves the degradation of the medicinal active substance, typically occurring on the surface of an anode.

Conclusions: As evident, there exist numerous methods for removing antibiotics from water, each with its own set of advantages and disadvantages. The selection of a particular method depends on factors such as the chemical structure of the pharmaceutical substance and the composition of the solution.

References:

[1] Phoon, B. L., Ong, C. C., Saheed, M. S. M., Show, P. L., Chang, J. S., Ling, T. C., Lam, S. S., & Juan, J. C. (2020). Conventional and emerging technologies for removal of antibiotics from wastewater. *Journal of Hazardous Materials*, 400, 122961.

SB-OP11 THE EFFECT OF POLYMERS TO OIL STORAGE ROCKS

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Abstract: *The polymer is the material that plays one of the most important roles in the application of recovery technology, and in particular speaking about surfactant polymers. Polymer injection can result in a significant increase in crude oil production in the recovery operation compared to conventional water injection techniques. One such process involves mixing and injecting the polymer over a longer period of time until about half of the reservoir's pore volume is injected. When water is injected into a reservoir, it follows the path of least resistance to flow, usually through high-permeability layers, by suction directly to the lower-pressure region of the production wells. If the crude oil in the reservoir has a higher viscosity than the injection water, the water will bypass it and the result will be lower flow efficiency and lower recovery.*

The purpose of polymer injection is to improve reservoir flooding efficiency and decrease mobility dynamics between water and crude oil, with the ultimate goal of a fairly equal mobility rate.

Key words: *oil enhanced, polymers, rocks*

Introduction: In enhanced technology, injection surfactant polymers (SP = Surfactant Polymer) are obtained by injecting a surfactant – most often a mixture of cosolvents, surfactants, stabilizers – to lower the interfacial tension to values of up to 10 mN/m. Sometimes it is necessary to use a water preflow to lower the salinity and especially the concentration of divalent ions in the deposit. This water preflow is followed by the injection polymer and surfactant which can be injected sequentially or simultaneously.

Hydrogel polymers to control the mobility of injected water have been used in this application for many years. These polymers are non-Newtonian fluids (also called pseudoplastics) because their viscosity is a function of shear rate. They are usually used with surfactants and alkaline agents to increase the efficiency of tertiary recovery.

Experimental and/or Modelling: Recent inventions that manage to meet the wide variety of conditions encountered in oil fields around the world include the following:

Polyacrylamides. A synthetic polymer - a variety of these are available through several manufacturers.

In general, the performance of a polyacrylamide will depend on its molecular weight and degree of hydrolysis. Partially hydrolyzed polyacrylamide (Partially hydrolyzed polyacrylamide, as a linear polymer, can be hydrolyzed. Hydrolysis can occur in an alkaline state, and the amide group becomes a carboxyl group), is one of the polyacrylamide group, having the form of a straight chain polymer of

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acrylamide monomers on which some of them has been hydrolyzed. The molecule is a flexible chain structure known as a random coil and is therefore a polyelectrolyte, which will interact with ions in solution.

Hydrogel polymers are the most commonly used polymers in oil recovery technology applications, especially due to the fact that it is relatively low in price with good viscosity properties and well-known physicochemical characteristics. Implementation of this technology is relatively easy and can significantly improve the crude oil recovery rate under standard reservoir conditions. This polymer is available in various molecular weights up to 30 million and can be used for temperatures up to 99℃ depending on water hardness.

Xanthan gum / Biopolymer. Xanthan gum is a polysaccharide or commonly referred to as a biopolymer. The structure is shown in Figure 30b. It is produced by the microbial action of Xanthomonascampestris on a carbohydrate medium substrate with a protein supplement and an inorganic nitrogen source. Biopolymer is an extracellular sludge that forms on the surface of cells. Xanthan gum is well known to perform well in high salinity waters. It is relatively compatible with most surfactants and other liquid injection additives used in tertiary crude oil recovery formulations.

Alkaline solutions of surfactant polymers (ASP). Components of Alkaline Surfactant Polymer Injection - Alkali Surfactant Polymer (ASP) injection is the injection of a solution containing polymer, alkaline solution and surfactant. Polymer injection is designed to increase volumetric thrust efficiency as well as displacement efficiency. The presence of alkaline substances and surfactants implies a special design for the recovery of residual crude oil.

Conclusions: The purpose of polymer injection is to improve the efficiency of reservoir flooding and decrease the mobility dynamics between water and crude oil.

References:

[1] Standnes, D. C., Skjevrak, I., 2014, *Literature review of implemented polymer field projects*. J. Pet. Sci. Eng. 122 (2011) 761-775

BOOK OF ABSTRACTS

SICHEM – 2024

C – Biomaterials and composites in chemical and biochemical applications (BCCBA)

1. Keynotes

SC-KN01 A PERSPECTIVE OF THE INTERPLAY BETWEEN KINETIC AND RELAXATION PHENOMENA IN LACTIC ACID-BASED POLYMERS

Mariana Cristea[1,*], Daniela Ionita[1]

[1]"Petru Poni" Institute of Macromolecular Chemistry, Aleea Grigore Ghica Voda 41A, Iasi, Romania

Abstract: *Lactic acid-based polymers are leaders in the field of renewable materials and present a challenging behavior regarding their thermo-rheologically behavior. This presentation will resume some relevant examples that will cover raw poly(lactic acid), biocomposites and lactide-based copolymers.*

Key words: poly(lactic acid), thermo-mechanical analysis, biocomposites

Introduction: The glass transition temperature (T_g) is regarded as a representative characteristic of polymeric materials, due to the fact it establishes the possible uses of polymers or the processing conditions. Furthermore, very often the rationale behind the structure-property relation of a polymer structure is founded on the values of T_g. and the question is how reliable is this approach. When other phenomena take place during heating and, even more, they overlap the process of glass transition, the thermo-rheological behavior will not follow a regular trend. It is the case of lactic acid-based polymers whose attributes (biocompatibility, controlled hydrolysis) recommended them for resorbable medical devices or environmentally degradable materials [1]. The presentation will focus on the particularities of this type of polymeric materials, as they resulted from advanced thermo-rheological investigations [2].

Experimental: The investigated samples will include raw PLA, biocomposites and lactide-based copolymers. Thermogravimetric analyses (TGA) were conducted on a Discovery TGA 5500 (TA Instruments), at 20 °C/min. Differential scanning calorimetry (conventional—DSC and modulated—MDSC) was performed with Discovery DSC 250 (TA Instruments). Isochronal (1 Hz, 2 °C/min) and multiplex (0.5, 1, 2, 5, 10 Hz) dynamic mechanical analysis (DMA) were carried out on PerkinElmer Diamond instrument and RSA G2 (TA Instruments), in tension and bending mode.

Results and discussions: Generally, the TGA results established the upper limit of the DSC investigations. From the entire experimental evidence (DSC, MDSC, DMA) a complex series of successive and overlapping phenomena were revealed as the samples are heated from 0 °C to over 150 °C (enthalpic relaxation, glass tramsition, cold crystallization, melting, welding). A pertinent visual proof that reveals the difference between the behavior of a conventional thermoplastic elastomer and poly(lactic acid) is schematically displayed as the storage modulus

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(E’) *vs.* temperature (T), the result of a DMA experiment (Fig. 1). The PLA material could have the second rubbery plateau before the melting. It is more a rule than an exception that the region B includes not only the glass transition (50-70 ^{o}C), but also the enthalpic relaxation (accompanied by shrinking) and the onset of cold crystallization.

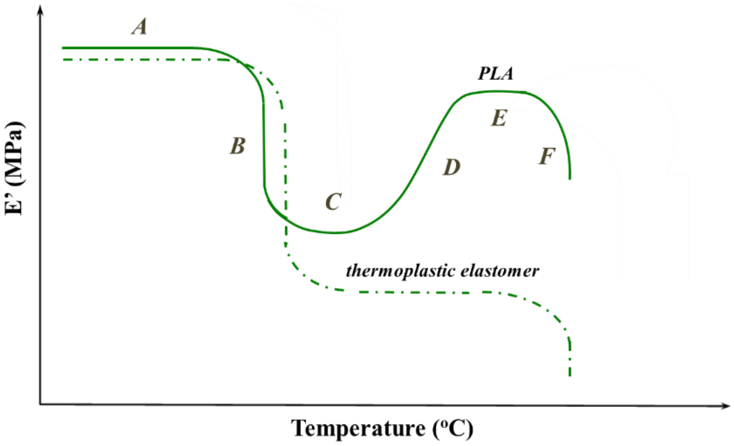

Fig. 1 Storage modulus E’ *vs.* temperature curves of a thermoplastic elastomer (non-continuous line) and an un-annealed PLA (continuous line): A-the glassy region, B-the glass transition region, C- the first rubbery plateau, D-the cold crystallization, E-the second rubbery plateau, F-the flowing region.

In the situation where the polymeric material is enough flexible, the plateau C does not occur and there is a sudden increase of E’, immediately after its drop. The contraction of the PLA material at the beginning of the F region may seem unusual, however it is associated with a welding process.

Conclusions: PLA-based polymers are unique for the whole hierarchy of phenomena that are developed in the range of temperature essential for practical applications.

References:

[1] Zhao X., Liu J., Li J., Liang X., Zhou W., Peng S., Strategies and techniques for improving heat resistance and mechanical performances of poly(lactic acid) (PLA) biodegradable materials, *Int. J. Biol. Macromol.* 218, (2022) 115-134.

[2] Cristea M., Ionita D., Iftime M.M., Dynamic mechanical analysis investigations of PLA-based renewable materials: How are they useful? *Materials* 13, 5302, (2020), 1-21.

SC-KN02 ENVIRONMENTAL IMPACT ON THE BUILDING MATERIALS OF ARCHAEOLOGICAL SITES

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[2] ICECHIM, Research Group "Evaluation and Conservation of Cultural Heritage", Bucharest

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Abstract: *Environmental effects on archaeological buildings from proximity of the marine area.*

Key words: archaeological buildings; environment; deterioration;

Introduction: This paper presents the results of scientific results on the conditions of deterioration that have affected archaeological buildings in the proximity of the marine environment. The factors of deterioration (mechanical, chemical and biological) from seawater and marine (or Danube) aerosol are studied on some monuments, such as: Basarabi-Murfatlar, Adamclisi, Roman Mosaico, Sacidava, as case studies, are investigated to verify their degradation conditions and weathering status.

Experimental and/or Modelling: Some techniques as: XRD, XRF analysis (for mineralogical compositions, lithotype and petrographic characteristics of stone samples), OM, SM, SEM (for the morphological characteristics of the same samples), FTIR, Raman (for the chemical composition of the involved structures). In addition, microbiological investigations will be presented to evaluate the colored hard crusts that affected the stone surfaces in these monuments.

Results and discussions: The obtained results demonstrated that the factors of severe damage influenced these monuments through chemical, mechanical and biological mechanisms. The mechanisms mentioned induce various effects in the material, including physical changes like abrasion and wear, as well as chemical transformations such as salt crystallization and formation of new minerals. The presence of black and colored biogenic hard crusts could indicate microbial activity or deposition of organic matter on the surface. Additionally, the techniques for monitoring some parameters: temperature and relative humidity, air quality (SO2, NOx, O3, PM10, PM2.5, etc.), will be presented and discussed. Salt crystallization as a major factor in the degradation of porous materials in the built heritage, provoque weathering effects, due to the presence of salt deposits that affects the rocks and artificial materials at the level of these monuments.

Conclusions: Different examination techniques are used to assess the current state of damage of some monuments, as well as the intermediate interventions.

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BOOK OF ABSTRACTS

SICHEM – 2024

C – Biomaterials and composites in chemical and biochemical applications (BCCBA)

2. Oral presentations

SC-OP01 HEMP FIBERS MODIFIED WITH GRAPHITE OXIDE AS GREEN AND EFFICIENT SOLUTION FOR WATER REMEDIATION

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Abstract: *A novel adsorbent based on GO-modified hemp fibres was designed and tested for removing methylene blue from aqueous solutions.*

Keywords: Hemp fibre, Water purification, Graphite oxide, Natural fibre, Adsorption, Advanced materials

Introduction: Traces of synthetic dyes in wastewater represent a great issue due to their impact on ecosystems [1]. Adsorption can be considered the most used methodology to remove them. The scientific community is focusing on the use of novel and sustainable adsorbents. Natural fibres have been selected to be a novel class of adsorbents. So, this work focuses on the design of graphite oxide (GO)-modified hemp fibres-based adsorbent for methylene blue removal.

Experimental*: Reagents:* Hemp fibres (HF), (3-Aminopropyl)triethoxysilane, NaOH, Methylene blue (MB) HCl solution 37% and graphite oxide. *Modification of HF:* HF were functionalized with (3-Aminopropyl)triethoxysilane through the formation of siloxane oligomers and subsequent functionalization with graphite oxide. *Adsorption tests:* Adsorption tests were performed in batch mode The concentration of MB was evaluated by using UV–Vis spectroscopy considering the absorbance at λ=664 nm.

Results and discussions: Adsorption tests were carried out to investigate the effect of pH, temperature, and initial dye concentration. Figure 1 shows the adsorption curves versus contact time (T=20°C) by varying the pH. On the right side, absorbance curves are shown while below the colorimetric variations of dye solution along time were reported.

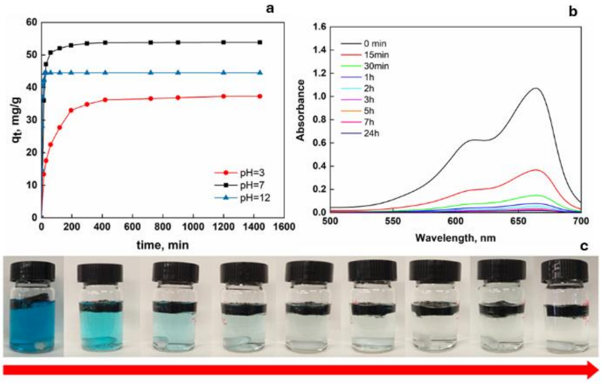

Fig. 1 qt versus time for adsorption of MB at different pH; b) absorbance curves of MB and c) colorimetric variations of dye solutions along time.

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The adsorption capacity (q_t, mg/g) increased with contact time. At low pH, H_3O^+ ions can compete with cationic MB ions. So, a reduction of adsorption capacity was observed. As pH overcomes the point of zero charge (6.35), an excess of negative charge on the surface adsorbent contributes to increase the adsorption capacity. Besides, at pH=12 lower values of q_t were recorded since the potential demethylation of MB [2]. As T raises, an increase in the removal efficiency occurred since the process is endothermic. Finally, as the initial dye concentration increase (from 5 to 35 mg/L) an increase in q_t was observed up to 372 mg/g.

Conclusions: The GO modified hemp fibers was used as novel and efficient adsorbent for MB removal from wastewaters showing adsorption capacity up to 372 mg/g.

References:

[1] Viscusi, G.; Lamberti, E.; Gorrasi, G., Hemp Fibers Modified with Graphite Oxide as Green and Efficient Solution for Water Remediation: Application to Methylene Blue, *Chemosphere*, 288, (2021**)**, 132614-132627.

[2] Batzias F.A., Sidiras D. K., Simulation of Dye Adsorption by Beech Sawdust as Affected by PH, *J. Hazard. Mater.*, 141, 3, (2007), 668–679.

SC-OP02 NANOTOPOGRAPHY CONTROL VIA ELECTROCHEMICAL ANODIZATION OF TITANIUM – ADVANCING BIOMEDICAL APPLICATIONS AND GREEN CHEMISTRY

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Abstract: *By controlling nanotopography via anodization, specific nanoscale morphologies are tailored and the* TiO_2 *coatings can be further functionalized for improving biointerfaces and multifunctionality. This work shows the significance of tailoring and modifying coatings for targeted applications and their biointerface interactions.*

Key words: Electrochemical anodization, Nanotopography, Nanoscale, Biomedical

Introduction: The modification of titanium and its alloys on the nanoscale level is a widely used technique in the field of biomedicine, impacting cell fate, and providing improved biocompatibility and corrosion resistance. The resulting nanoscale topography features a well-controlled surface, high aspect ratio, and high surface area, making it an ideal material for various applications that require functionality [1,2].

Experimental: Electrochemical anodization is performed in a two-electrode electrochemical cell in organic-based electrolytes containing fluoride ions at 58V, 2.5h (30V, 4h) or 1M phosphoric acid at 20V, for 30min. The morphology and chemical composition of the samples are evaluated by SEM, EDX, and XPS, and hydrophilicity by contact angle measurements.

Results and discussions: In the context of biomedical research, there is a focus on enhancing osseointegration, reducing the inflammatory response, promoting antibacterial activity, and developing applications such as biosensors and drug delivery systems. These efforts are based on a well-established control of nanotopography, with TiO_2 nanostructures providing exceptional control in the sub-100 nm range. Anodization results in various nanoscale morphologies, such as electropolished surfaces, compact oxide structures, nanopores, nanotubes, and mesoporous layers [1–5]. Fig. 1 shows a typical anodization setup, with the resulting compact, nanotubular or spike morphology.

Moreover, the TiO_2 coatings can be functionalized with a secondary material, e.g., nanoparticle, graphene/graphene oxide flakes or coatings, hydroxyapatite, to improve the biointerface or to achieve multiple functionalities on the same material surface (anticorrosion, therapeutic functions, antifouling, etc.).

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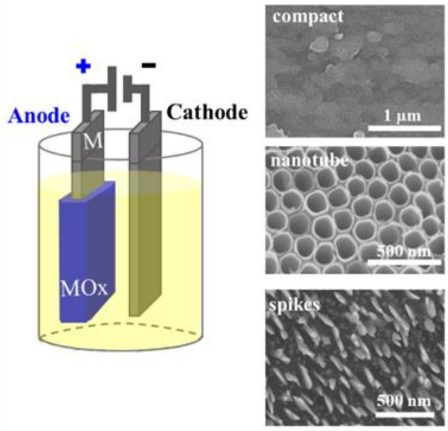

Fig. 1 Electrochemical anodization setup and example of various morphologies obtained (compact, nanotubes, spikes)

Conclusions: Here we show the key aspects for tailoring coatings obtained by electrochemical anodization, with a compact, porous or nanotubular morphology and their further modification for targeted applications. More importantly, the changes occurring at the interfaces and further influence on the biointerface are also discussed.

References:

[1] K. Lee, A. Mazare, P. Schmuki, One-Dimensional Titanium Dioxide Nanomaterials: Nanotubes, Chem. Rev. 114 (2014) 9385–9454. https://doi.org/10.1021/cr500061m.

[2] J. Park, A. Cimpean, A.B. Tesler, A. Mazare, Anodic TiO2 Nanotubes: Tailoring Osteoinduction via Drug Delivery, Nanomaterials. 11 (2021) 2359. https://doi.org/10.3390/nano11092359.

[3] A. Mazare, Comment on “old is Gold: Electrolyte Aging Influences the Topography, Chemistry, and Bioactivity of Anodized TiO2Nanopores,” ACS Appl. Mater. Interfaces. 14 (2022) 14837–14841. https://doi.org/10.1021/acsami.1c18860.

[4] J. Park, A.B. Tesler, E. Gongadze, A. Iglič, P. Schmuki, A. Mazare, Nanoscale Topography of Anodic TiO 2 Nanostructures Is Crucial for Cell–Surface Interactions, ACS Appl. Mater. Interfaces. 16 (2024) 4430–4438. https://doi.org/10.1021/acsami.3c16033.

[5] A.B. Tesler, S. Kolle, L.H. Prado, I. Thievessen, D. Böhringer, M. Backholm, B. Karunakaran, H.A. Nurmi, M. Latikka, L. Fischer, S. Stafslien, Z.M. Cenev, J.V.I. Timonen, M. Bruns, A. Mazare, U. Lohbauer, S. Virtanen, B. Fabry, P. Schmuki, R.H.A. Ras, J. Aizenberg, W.H. Goldmann, Long-term stability of aerophilic metallic surfaces underwater, Nat. Mater. (2023). https://doi.org/10.1038/s41563-023-01670-6.

SC-OP03 FORMULATION AND CHARACTERIZATION OF BACTERIAL CELLULOSE-BASED ICECREAM

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Abstract: *Ice-cream is one of the most popular frozen desserts in the whole word. New innovative food products were developed based on cow milk and bacterial cellulose (BC) as ice cream formulations. Bacterial cellulose (BC) produced extracellularly by different Gram-negative bacterial cultures of Gluconacetobacter, Acetobacter, Agrobacterium, etc. has proven to be one of the purest forms of cellulose and an important fibre source in food products from Thailand and Indonesia [1]. Its high-water retention capacity (98% wt.) and enhanced biocompatibility makes it an interesting as a possible prebiotic compound. In this study, 3 dairy ice cream formulations with different concentrations of BC were proposed as food products with prebiotic function. The non-frozen formulations were characterized by rheological properties. The final products were characterized by texture, firmness, density, chemical composition, melting point.*

Key words: bacterial cellulose, ice-cream formulation, rheological properties, melting point, texture, firmness

Introduction: Bacterial cellulose (BC), derived from aerobic fermentation of sugars or fruit wastes, is highly valued for its diverse applications in engineering, medical devices, and food products [1]. Its fibrous structure and remarkable water retention capacity make it ideal for enhancing texture and extending shelf life in food formulations [1]. This study focuses on designing and characterizing ice-cream formulations incorporating BC at concentrations of 1%, 3%, and 5% wt. aiming to understand the impact of BC concentration on ice cream properties, paving the way for the development of innovative frozen desserts with improved texture and thermal stability.

Experimental and/or Modelling: *Reagents* Commercially available ingredients used for ice-cream formulations included milk (3.5% lipid content, Danone, Romania), cocoa (Dr. Oetker, Germany), sugar (Furnicuța, Romania), liquid cream (35% lipid

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content, LaDorna, Romania), and salt (Olympia, Romania). *Production of BC:* BC membranes were obtained by static culture in Mass Transfer Laboratory of Politehnica Bucharest according to the method described elsewhere [2] followed by sterilization and dehydration up to 10-12% wt moisture content. The resulted fibres were dispersed in the classical milk-based ice-cream mixture by Thermomix equipment (TM6 Vorwerk), followed by maturation and freezing. The samples were encoded IC (for classical blank formulation), ICBC1, ICBC3, and ICBC5 for samples modified with 1, 3, respectively 5% wt concentration of BC.

Results and discussions: The non-frozen mixture's viscoelastic behavior transitioned from resembling a Bingham fluid in the IC blank sample to aligning more closely with the Herschel-Buckley model, as evidenced by the values of R^2 approaching unity for the ice cream formulation containing 5% weight BC (ICBC5). **Table 1** presented the results in terms of firmness, cohesivity, elasticity and gumminess of all samples indicating a slight increase of firmness, elasticity and gumminess as the concentration of BC increased.

Tabel 1. *Texture analysis of blank and BC-based formulations*

Sample	Firmness (Force 40 %) (N)	Cohesivity	Elasticity	Gumminess (N)
IC	0,02 ± 0	0,94 ± 0,04	0,97 ± 0,02	0,02 ± 0
ICBC1	0,02 ± 0	0,78 ± 0,02	0,99 ± 0,01	0,02 ± 0
ICBC3	0,04 ± 0	0,59 ± 0,04	0,98 ± 0	0,03 ± 0
ICBC5	0,04 ± 0	0,61 ± 0,07	1 ± 0,02	0,03 ± 0

Reduced cohesivity was registered as the BC content increased, this being attributed probably to high fat content or the higher water content retained by the BC fibers that slightly prevents the formation of a compact structure.

Conclusions: Thus, the results obtained for BC-based ice cream formulations represent a good premise for dessert products with possible prebiotic role.

References:

[1] Andriani, D., Apriyana, A.Y. & Karina, M. The optimization of bacterial cellulose production and its applications: a review, *Cellulose* 27, (2020) 6747–6766.

[2] Rusen, E., Isopencu, G., Toader, G. et al. Improved degradability and mechanical properties of bacterial cellulose grafted with PEG derivatives, *Cellulose* 30, (2023) 4293–4314.

SC-OP04 PRELIMINARY EXPERIMENTAL RESEARCH TO OBTAIN CERAMIC MATRIX COMPOSITES BY USING CHEMICAL VAPOR REACTION TO BE USED AS GAS TURBINE BLADES

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Abstract: *Owners and operators are seeking cost effective ways to: expand gas turbine's performance and operability, improve efficiency, gain more output and extend the lifespan of their existing equipment, thus, minor turbine improvements to existing equipment, is a more attractive option.*

Gas turbine blades made of ceramics are the next development step in the field of aviation and industrial turbo engines because they allow reaching performances (e.g. increased effectiveness and delivered power, low specific consumption, etc.) superior to the existing ones that uses metallic blades. Currently, ceramic matrix composites (CMC) are classified in terms of fibers and matrix materials, separated by slash (e.g. C/SiC is a CMC made of silicon carbide matrix and carbon fibers as filler)

The paper is presenting the experimental work for obtaining a Silicon Carbide based ceramic matrix composite starting from a composite material made of carbon fibers and two different resins: epoxy and phenol. The aim of the research was to obtain silicon carbide starting from organic materials: carbon fiber and resins by thermochemical reaction of these materials and gaseous Silicon. Firstly, the organic matrix was thermally treated in inert gas in order to eliminate all the volatiles but to keep the carbon within the matrix. Secondly, the obtained carbonized material was thermally treated in vacuum and in the presence of gaseous Si in order to form SiC.

The source of gaseous silicone monoxide can be produced by two different powder mixtures which are heated at 1600˚C. First, by a reaction among 60%SiC+30%Si+10%Al2O3 called mixture 1 and second by the reaction of 50%SiO2+50%Si called mixture 2, both of them being prepared by co-milling in a planetary mill for 30 min and drying for 12 h at 180˚C. Mixture 1 is put in a carbon crucible and Cf/C composite is placed inside the powder mixture in a furnace in vacuum atmosphere and heated at temperatures from 1600˚C for 3 hours with a heating rate of 10˚C/min. Mixture 2 is placed in an alumina crucible and the Cf/C composite is placed above the mixture without contact with the powder. Mixture 2 is placed in a furnace in vacuum atmosphere and heated at 1600˚C for 3 hours with a heating rate of 10˚C/min.

The obtained materials were characterized from mechanical and optical point of view in order to assess their properties.

The main findings of the research are focused on the transformation of carbon-based matrix in SiC and also highlights the next steps to be taken and the adjustments to be made in order to obtained the proposed result.

Key words: ceramic matrix composite, chemical vapor reaction, carbon fiber, gas turbine

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SC-OP05 BIODEGRADABLE BIOPOLYMER FOR SUPPORTED BIODEGRADABLE CATALYST IN TRANSESTERIFICATION TO ALKYL ESTERS

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Abstract: *Biopolymers have versatile functional groups that can successfully participate in the binding of chemical compounds, resulting in matrices with special properties in terms of chemical stability or functionality. One such biopolymer, bacterial cellulose (BC), was used in this work to support guanidine as a strong alkaline biodegradable compound to further heterogeneously catalyze the transesterification reaction to alkyl esters, obtaining an ester content of 91–95% in the conversion of vegetables used. oils.*

Key words: biodegradable polymer, biodegradable supported catalyst, transesterification, alkyl esters

Introduction: Biodiesel has properties similar to classic diesel and characteristics that can recommend it as an alternative or in addition to petro diesel. The low percentage of biodiesel regulated and already used, B6 or B7 (6 or 7% biodiesel and 93 or 94% petrodiesel) can easily be increased to B20, B30 or even B50, thanks to the latest research that shows that any lipids - containing waste can be converted into alkyl esters. These wastes are in huge quantities in any community, come from multiple sources and can provide raw materials for a capacity between 0.1-200000 t/year [1-3]. Waste vegetable oil was used in this work to test the supported catalyst.
Experimental: *Reagents:* The following raw materials were used in this experimental research: dimethyl sulfate, urea, methanol, 25% ammonia solution, potassium hydroxide pellets, waste sunflower cooking oil (household). Procedure: The synthesis of guanidine was carried out in three steps, starting from urea and dimethyl sulfate, molar ratio 1:1, with successive reactions of methylation, ammonolysis (preceded by neutralization) and precipitation. The resulting guanidine was kept bound to methanol. To prepare the catalytic support, the obtained bacterial cellulose was previously subjected to thermal and chemical treatment: neutralization with 0.1 M KOH solution and left in methoxide for several days, then dried and finally functionalized by the methanolic guanidine impregnation method.

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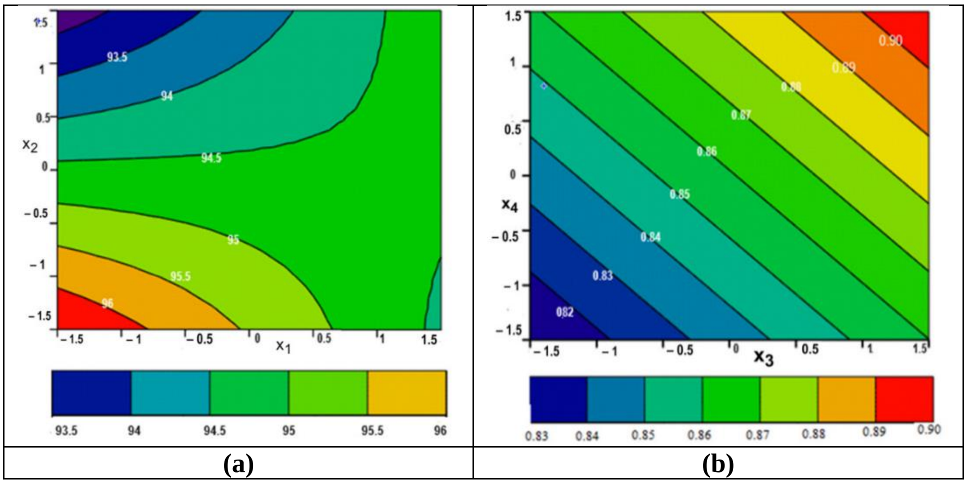
Results and discussions: For a 2^4 factorial experimental design, a response y dependent on the four factors was expressed according to equation (1), where x_i are the dimensionless process factors. These dimensionless factors are defined by equation (2), where they have the values $+1$ and -1. For transesterification of used vegetable oils using BC_{KOH}/Guanidine as a catalyst, the experimental investigation concerning the factors that influence the transesterification yield after esters and after glycerin is presented in figure 1.

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \sum_{i=1}^{4} \beta_i x_i + \sum_{i=1}^{4} \sum_{j=i+1}^{4} \beta_{ij}\, x_i x_j + \\ + \sum_{i=1}^{4} \sum_{j=i+1}^{4} \sum_{k=j+1}^{4} \beta_{ijk} x_i x_j x_k + \beta_{1234} x_1 x_2 x_3 x_4 \qquad (1)$$

$$x_i = \frac{z_i - z_{iC}}{\Delta z_i} = \frac{z_i - \frac{z_{i,max} + z_{i,min}}{2}}{\frac{z_{i,max} - z_{i,min}}{2}}, \quad i = 1 \ldots 4 \qquad (2)$$



(a) **(b)**

Fig. 1. Dependence of transesterification: (a) after esters on factor x_1 and x_2 for x_3=x_4=0; (b) after esters on factor x_3 and x_4 for x_1=x_2=0

Conclusions: In this experimental investigation, a supported catalyst was first constructed and then tested in transesterification, where it was able to concert triglycerides producing over 95% methyl ester.

References:

[1] Răducanu, C.E.; Dobre, T.; Mihăiescu, D.E.; Moroşan, A.; Jidveian, R.; Cioroiu Tîrpan, D.R.; Vasiliu, A.D.; Gogoaşă, C.I.; Pârvulescu, O.C.; Trică, B. Synthesis of Guanidine and Its Deposition on Bacterial Cellulose as Green Heterogeneous Catalyst for Transesterification to Methyl Esters, *Energies*, 17, 2024, 1344.

[2] Ameen, M., Ahmad, M., Zafar, M., Munir, M., Mujtaba, M.M., Sultana, S., Rozina, El-Khatib, S.E., Soudagar, M.E.M., Kalam, M.A., Prospects of Catalysis for Process Sustainability of Eco-Green Biodiesel Synthesis via Transesterification: A State-Of-The-Art Review. *Sustainability*, 14, 2022, 7032.

SC-OP06 HIGH ENTROPY PEROVSKITE OXIDES: EXPLORING A PARADIGM FOR PROMISING MATERIALS

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Abstract: *Perovskites are probably one of the most studied families of oxides with a wide array of functional properties such as: superconductor, ferroelectric, colossal magnetoresistance, multiferroic, high permittivity insulator, low permittivity insulator, conductor, thermoelectric, and ferromagnet. Current design strategies for perovskite oxides involve chemical modification at different crystallographic sites, chemical additives that do not target lattice sites and novel processing approaches dedicated to bulk ceramics, think and thin films. An alternative approach which has recently attracted the scientific community's attention refers to the concept of high-entropy configuration. Compositional design by this approach may lead to unexpected properties caused by a random distribution of species in crystalline structures. This study explores a novel lead-free A-site high-entropy* ABO_3 *perovskite oxide and the correlation between atomic-size differences, Goldschmidt tolerance factor and microstructural features on the electrical behavior of the ceramics. Oxide powders of* $Bi_{0.2}K_{0.2}Ba_{0.2}Ca_{0.2}Sr_{0.2}TiO_3$ *nominal composition were prepared by a Pechini method with the aim to obtain narrow particle size distribution and homogeneous distribution of the elements in the particles. The particle obtained in the optimum conditions were of 16-18 nm and consisted of a mixture of cubic, tetragonal and orthorhombic perovskite polymorphs. Processing of ceramics at different temperatures leads to differences in microstructures (grain size, density), which ultimately affects the electrical behavior. Detailed characterization of the dielectric properties illustrates a ferroelctric-relaxor crossover dependent on the microstructure. The thermally stable dielectric response of lead-free high entropy ceramics, with low permittivity and dielectric losses over a wide temperature range, indicates that adjusting the composition through high-entropy design and the microstructure through appropriate synthesis processes significantly affects their electrical behavior, expanding their use in electronic applications.*

Key words: high entropy ceramics; perovskite; realxor; Pechini method.

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SC-OP07 SYNTHESIS AND FUNCTIONALIZATION OF BIOACTIVE GLASS AND MCM-41 FOR BIOMEDICAL ENGINEERINGS

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Abstract: *The synthesis methods involve obtaining two biomaterials, mesoporous silica particles and bioactive glass particles, for tissue engineering purposes.*

Key words: bioactive glass, MCM-41, sol-gel synthesis.

Introduction: Bioactive glass and MCM-41 are both highly versatile materials that are widely used in biomedical research and applications. Bioactive glass is known for its ability to stimulate bone regeneration by facilitating hydroxyapatite formation, whereas mesoporous silica, typified by MCM-41, has exceptional proficiency in encapsulating therapeutic agents, being highly desirable for drug delivery applications, especially in hard tissue engineering.

Experimental: MCM-41 and bioactive glass were synthesized using the sol-gel method. The experimental procedures involved the utilization of CTAB as a template, which was dissolved in a water-solvent mixture. Subsequently, the necessary precursors were gradually added under constant stirring. The reaction mixture was left to stir at room temperature for 24 hours prior to filtration, drying and calcination. Physicochemical characterization of the mesoporous materials was conducted using BET porosimetry, FT-IR spectroscopy and X-ray diffraction.

Results and discussions: In the present work, mesoporous particles were synthesized using sol-gel technique, and procedural adjustments were made to produce materials with diverse textural properties. Their high surface area together with their interlinked pore network, make them suitable candidates for doping and loading with metal ions, which can enhance their biocompatibility or even to induce new properties such as antimicrobial activity.

Conclusions: The synthesis of bioactive glass and MCM-41 holds significant promise for biomedical applications. These materials offer unique properties that can benefit drug delivery and tissue engineering. Further research will focus on doping / loading mesoporous materials with metal ions using different methods [4].

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References:

[1]. Cannio, M, Bellucci D, Roether JA, Boccaccini DN, Cannillo V. Bioactive Glass Applications: A Literature Review of Human Clinical Trials. Materials. 2021; 14(18):5440.

[2] A.R. Farmani, M.A. Salmeh, Z. Golkar, A. Moeinzadeh, F.F. Ghiasi, S.Z. Amirabad, M.H. Shoormeij, F. Mahdavinezhad, S. Momeni, F. Moradbeygi, J. Ai, J.G. Hardy, A. Mostafaei, Li-Doped Bioactive Ceramics: Promising Biomaterials for Tissue Engineering and Regenerative Medicine, J Funct Biomater 13(4) (2022).

[3] N. Kütük, Mesoporous silica nanoparticles, methods of preparation and use of bone tissue engineering, International Journal of Life Sciences and Biotechnology 4(3) (2021) 507-522.

[4] G. Dolete, B Purcăreanu, D.E. Mihaiescu, D Ficai, O.-C. Oprea, A.C. Bîrcă, C Chircov, B. Ș. Vasile, G Vasilievici, A Ficai and E Andronescu; A Comparative Loading and Release Study of Vancomycin from a Green Mesoporous Silica; Molecules 2022, 27(17), 5589; https://doi.org/10.3390/molecules27175589

BOOK OF ABSTRACTS

SICHEM – 2024

C – Biomaterials and composites in chemical and biochemical applications (BCCBA)

3. Poster presentations

SC-P01 MANUFACTURING ROUTES OF POROUS STRUCTURES BASED ON MERWINITE WITH APPLICABILITY IN REGENERATIVE TISSUE ENGINEERING

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Abstract: *With the growing demand for ideal materials for bone grafting, magnesium silicates have come to the attention of many researchers for applications in tissue engineering, calcium and silicon being two ions directly involved in the biological processes underlying bone regeneration. In this study, a calcium and magnesium silicate, namely merwinite (MW), was produced by sol-gel synthesis, being presented comparatively alongside a zinc-doped alternative of the base material (MW-Zn). The study proposes four different routes to obtain unitary or composite structures that can help patients with bone defects to rehabilitate the function of damaged tissue and stimulate the regeneration of damaged hard tissue following various pathologies. One of the manufacturing routes addressed consists in making compact or porous products obtained after the uniaxial pressing of precursor oxide powders mixed with a porogenic agent that gives the ceramic matrix after sintering the internal structure of hard bone, favouring the adhesion of cells to the implanted substrate. Additive manufacturing is a method of great interest and relevance in the field of bioengineering, being used to obtain customized products with a controlled porosity. In this technique, the precursor powders were mixed with hydroxypropyl methylcellulose (HPMC), an inert polymer with high biocompatibility, to form pastes used in the 3D printing process. At the same time, composite materials based on bacterial cellulose (BC) and MW/MW-Zn were made by ultrasound irradiation, resulting in three-dimensional porous hybrid materials. BC acts as a template with the role of favouring the formation of apatitic phases on the surface of the obtained structures, favouring cell proliferation. The present work also reports the synthesis and characterization of polycaprolactone (PCL)-based fibres loaded with MW/MW-Zn to form composite materials with bioactive properties and bioresorbability characteristics. Based on the FT-IR, EDX, SEM, XRD, DSC-TG analyses and the porosity analysis method proposed by Arthur, together with the mechanical resistance testing, the four types of materials obtained were characterized and studied, and together with the methods of biocompatibility analysis will complete their evaluation for use in tissue reconstruction and regeneration applications.*

Keywords: merwinite, sol-gel, porogenic agent, additive fabrication, bacterial cellulose, electrospinning, tissue engineering.

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SC-P02 ENVIRONMENTALLY RESPONSIBLE POLYURETHANE FORMULATIONS AS ALTERNATIVES TO HTPB BINDER USED IN COMPOSITE PROPELLANTS

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Abstract: *Polyurethanes produced from commercial polyether-based polyols or an experimental polyol based on polyethylene terephthalate (PET) recycled through glycolysis have been comparatively studied against hydroxyl-terminated polybutadiene (HTPB), a widely used binder in composite propellants for civil and military rockets with the aim of finding an environmentally friendlier alternative to the latter.*

Key words: PET recycling, Polyols, Polyurethane, Composite propellants

Introduction: Polyurethane is one of the most versatile polymers**[1]**, its thermo-mechanical properties being highly adjustable by different methods: altering the chain length, the degree of crosslinking, the ratio of soft/hard segments and by using different types of polyols/isocyanates. The polyols used in the synthesis of polyurethanes can be derived from "greener" sources such as vegetable feedstock (oils, lignocellulosic mass, proteins etc.) or by chemical recycling through the process of glycolysis of various polymers that have reached end-of-life, such as polyesters, polyamides or polyurethanes. Polyethylene terephthalate (PET) is one of the most used polymers**[2]** and the most common polyester**[3]**. Being such a high volume polymer that is also feasible for recycling through glycolysis, it is an attractive alternative for the production of polyols intended for polyurethane synthesis.

Experimental: Reagents: HTPB, commercial polyols based on polypropylene glycol, the experimental polyol RC3r based on PET glycolysis, glycerol as crosslinking agent, Isophorone diisocyanate (IPDI), dibutyltin dilaurate (DBTDL) as gelling catalyst and BYK®-1796 antifoaming additive. 8 polyurethane samples have been prepared employing four types of polyol (HTPB, Petol® 28-2LM, Petol® 56-3 and RC3r) and IPDI. Two ratios of NCO/OH and different amounts of glycerol were used.

Results and discussions: The synthesized polyurethanes were chemically, thermally and mechanically analyzed. FTIR spectra revealed urethane-specific

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groups. The polyurethanes synthesized using commercial polyols and the experimental polyol have shown improved mechanical properties compared to the HTPB-based polyurethane.

Conclusions: From the preliminary results, it can be concluded that the environmentally-responsible polyurethanes synthesized using commercial polyether polyols and the polyol RC3r made by chemical recycling of PET can be viable alternatives to the petroleum-based HTPB binder used in composite propellant rockets.

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References:

[1] J. Akindoyo, M. Beg, S. Ghazali, M. Islam, N. Jeyaratnam, Y. A. R., Polyurethane types, synthesis and applications-a review, RSC Adv 6 (2016) 114453–114482. https://doi.org/10.1039/C6RA14525F.

[2] Plastics - the Facts 2022 • Plastics Europe, Plast. Eur. (n.d.). https://plasticseurope.org/knowledge-hub/plastics-the-facts-2022/ (accessed February 28, 2024).

[3] L.W. McKeen, Chapter 6 - Polyesters, in: L.W. McKeen (Ed.), Fatigue Tribol. Prop. Plast. Elastomers Second Ed., William Andrew Publishing, Oxford, 2010: pp. 99–147. https://doi.org/10.1016/B978-0-08-096450-8.00006-5.

SC-P03 INTERPENETRATING POLYMER NETWORK HYDROGELS CONTAINING LDH, FOR THE CONTROLLED RELEASE OF INULIN

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***Abstract:** New composite interpenetrating polymer network hydrogels based on polyethylene glycol diacrylate, chitosan and hydrotalcite dopped with inulin were prepared with the aim of possible slow release of bioactive substances.*

Key words: PEGDA, Chitosan, hydrogels, LDH, inulin

Introduction: Lately, with the rapid development of industry, hydrogels have attracted more and more attention due to their large specific surface area and unique structure. Hydrogels are three-dimensional network-structured polymer formed by a polymer main chain and a hydrophilic functional group through covalent bonds, hydrogen bonds, or physical winding cross-linking [1]. Hydrogels have particular interest in tissue engineering and controlled drug delivery due to their high water content, permeability to oxygen and nutrients, and tissue-like elastic properties [2]. Although physically cross-linked natural hydrogels have been widely used for biomedical applications, chemically cross-linked hydrogels offer better control over their ultimate physical, structural and mechanical properties [3]. In addition, some gelation reactions can be performed under very mild conditions, such as in aqueous media, at room temperature, at body pH and even in situ, in a minimally invasive manner.

Experimental: For the development of the aimed hydrogels chitosan (CS) and polyethylene glycol diacrylate (PEGDA) were used. The solutions of the natural polymer and of the PEGDA macromonomer, in aqueous solutions of acetic acid, were mixed, followed by the addition of double layered hydroxides (LDH) or LDH imbibed with inulin. The crosslinking polymerization of PEGDA inside the CS network was initiated with the redox system composed from ammonium persulfate (APS) and tetramethylethylenediamine (TMEDA), at 37 °C, during 24 hours.

Results and discussions: In order to highlight the properties of the new developed hydrogels, the samples were characterized using various modern techniques such as FTIR, SEM and swelling degrees. FTIR spectra confirmed the occurrence of characteristic bands for the involved raw materials. The SEM images and swelling degrees confirmed the structure of interpenetrating network composite hydrogels.

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Conclusions: The aimed hydrogels based on CS and PEGDA were successfully developed and characterized by FTIR, SEM and also by their swelling degree capacity variation in time, indicating the possibility to be used for the slow release of inulin.

Aknowledgement: The study was funded by the Ministry of Education and Research through Executive Unit for Financing Higher Education, Research, Development and Innovation (UEFISCDI), grant. No. 646 PED/2022 DUACTIVMER and grant no. PN 23.06.01.01 AQUAMAT

References:

[1] Wang R., Zhang X., Zhu J., BaI J., Gao L., Liuc S., Jiao T., Facile preparation of self-assembled chitosan-based composite hydrogels with enhanced adsorption performances, *Colloids and Surfaces A* 598 (2020) 124860.

[2] Peppas N. A., Hoffman A S., Hydrogels, 153-155

[3]. R. Jayakumar et al., Biomedical applications of chitin and chitosan-based nanomaterials—A short review, Carbohydrate Polymers, 82,2010, p. 227-232.

SC-P04 EFFECT OF SURFACE ROUGHNESS OF CO-CR ALLOY MODIFIED BY HYDROXYAPATITE COATING

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Abstract *The effects of roughness on cobalt-chromium-molybdenum substrate were investigated in order to improve the quality of hydroxyapatite (HA) coating as well as enhance the cell responses. Blasting process used to roughing the substrates surface by using a different alumina particles size (19, 45, 110, and 250) µm then coated with HAp using sol-gel coating by spin coating technique. Analysis of surface morphology, crystal structure and chemical composition of surface with HA coating were analyzed using field-emission scanning electron microscopy and characterized by energy dispersive X-ray spectroscopy. However, the bioactivity and stabilization of thin films were analyzed by immersing implants in the simulated body fluid(SBF) then analyzed by scanning electron microscopy and characterized by X-ray spectroscopy to investigate the transformations in surface morphology and crystal structure after 7, 14, 21 days.*

Key words: Hydroxyapatite, Co-Cr alloy, X-ray spectroscopy, SEM, Thin film.

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SC-P05 DESIGN OF NANOVEHICLES LOADED WITH SENOMORPHIC DRUGS FOR TARGETTING SENESCENT CELLS

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Key words: liposomes, luteolin, drug delivery, senescent cells

Introduction: Cellular senescence is involved in different age-related diseases, eg. metabolic disorders, osteoporosis, cancer, neurodegenerative diseases, etc. Senescent cell targeting has become a viable treatment approach to slow down aging-related decline and lengthen life [1, 2]. Natural flavonoid luteolin is widely found in fruits and vegetables and has strong senomorphic effects that can alter important signaling pathways that control senescence [1]. The aim of this paper was the obtaining and characterization of liposomes and nanoparticles encapsulating luteolin, as senomorphic agent.

Experimental: The liposomes loaded with luteolin were obtained by thin-film hydration followed by sonication method, while luteolin-loaded nanoparticles were prepared using pullulan acetate as polymeric matrix via nanoprecipitation. The physico-chemical properties of the luteolin-loaded liposomes and luteolin-loaded nanoparticles including size and polydispersity index and entrapment efficiency, were evaluated using dynamic light scattering and UV-VIS spectrophotometry.

Results and discussions: Luteolin-loaded liposomes and luteolin-loaded nanoparticles exhibited a nano-size and narrow polydispersity index, and good entrapment efficiency (>75%). Additional in vitro research is necessary to assess the efficacy of luteolin-loaded liposomes in targeting senescent cells.

Conclusions: The findings of this study underscore the potential of luteolin-based formulations as senomorphic agents, offering new avenues for combating age-related ailments and promoting healthy aging.

Aknowledgement: This work was suported through the "Nucleu" Program, Contract no. 1N/2023, Project code PN 23-28 carried out with the support of MCID, project no. PN 23-28 03 01.

References:

[1] Zhang, L., Pitcher, L. E., Prahalad, V., Niedernhofer, L. J., & Robbins, P. D. (2023). Targeting cellular senescence with senotherapeutics: senolytics and senomorphics. *FEBS J.*, 290(5), 1362–1383. https://doi.org/10.1111/febs.16350

[2] Chaib, S., Tchkonia, T., & Kirkland, J. L. (2022). Cellular senescence and senolytics: the path to the clinic. *Nat. Med.*, 28(8), 1556–1568. https://doi.org/10.1038/s41591-022-01923-y

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SC-P06 SYNTHESIS, CHARACTERIZATION AND DFT STUDIES OF SOME PYRIMIDINE COMPOUNDS WITH THERAPEUTIC APPLICATIONS

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Abstract: *New pyrimidinone compounds with antimicrobial properties were synthesized.*

Key words: tetrahydropyrimidines, Biginelli reaction, antimicrobial activity, DFT analysis.

Introduction: Heterocycles are very used in medicinal chemistry, materials chemistry, and also as agents with therapeutic properties. Thus, Nifedipine is a pyrimidinone with pharmaceutical properties, used as antihypertensive and calcium channel blocker agent. Also, Monastrol, also a pyrimidinone, is used as anticancer agent. Starting from these applications, we used multicomponent reactions to obtain pyrimidinones as potent pharmaceutical agents [1-2].

Experimental and/or Modelling: *Synthesis* of heterocycles was carried out using multicomponent reactions. *All reagents were purchased* from Sigma Aldrich. Synthetic method uses the classic refluxing of the three-component with magnetic stirring and monitoring the reaction through thin layer chromatography. NMR spectra were performed on a Varian Inova-400 (500 MHz), in dimethyl sulfoxide (DMSO-d_6) [3-5]. All synthesized pyrimidinones were evaluated by qualitative and quantitative methods against two microbial strains [6-7].

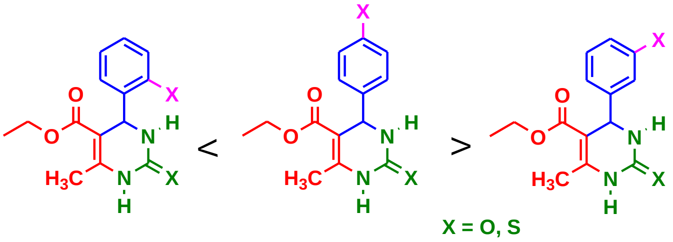

Fig. 1. Antimicrobial activity correlated with the position of the substituent on the benzene ring

Results and discussions: *Synthesis* of pyrimidinones was carried out using Biginelli reaction, starting from three components: ethyl acetoacetate, urea/ thiourea and various aldehydes. By optimizing the parameters of reactions (reaction time, solvent, catalyst) the compounds were obtained in good yields (70-80%). All compounds have shown good and very good antimicrobial activity, on all microbial strains tested. The structures of the synthesized pyrimidinones were optimized

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using the GAMESS 2012 software to perform a DFT analysis of the molecules and to found frontier molecular orbitals HOMO-LUMO. It has been found that the presence of nucleophilic group and the symmetry of one molecule and are key parameters for a good antimicrobial activity.

Conclusions: Correlating the antimicrobial activities of the compounds with their structures, showed that the presence of first-order substituents in *para* position of the aromatic ring leads to a high biological activity, compared to the presence of the same substituents in the *ortho* or *meta* positions. The observation was correlated with the calculated DFT parameters and HOMO-LUMO gaps (Fig. 1).

References:

[1] Marinescu, M. Biginelli Reaction Mediated Synthesis of Antimicrobial Pyrimidine Derivatives and Their Therapeutic Properties, *Molecules*, 26, (2021), 6022.

[2] Marinescu, M. Synthesis of Antimicrobial Benzimidazole–Pyrazole Compounds and Their Biological Activities, *Antibiotics*, 10 (2021), 1002.

[3] Potmischil, F., Deleanu, C., Marinescu, M., Gheorghiu, D. Hydroacridines - Part 23. ^{1}H and ^{13}C NMR spectra of *sym*-octahydroacridine, its 9-(3-pyridyl) and 9-(4-pyridyl) derivatives and the corresponding N(10)-oxides. An experimental approach to the diamagnetic anisotropy of the pyridine nucleus, *Magn. Res. Chem*., 40, 3, (2002), 237-240.

[4] Potmischil, F., Marinescu, M., Nicolescu, A., Deleanu C., Hillebrand, M. Hydroacridines: part 29. ^{15}N NMR chemical shifts of 9-substituted 1,2,3,4,5,6,7,8-octahydroacridines and their N-oxides, *Magn. Res. Chem.*, 46, 12, (2008), 1141-1147.

[5] Potmischil, F., Marinescu, M., Nicolescu, A., Deleanu, C. Hydroacridines: part 30. ^{1}H and ^{13}C NMR spectra of 9-substituted 1,2,3,4,5,6,7,8-octahydroacridines and of their N-oxides, *Magn. Res. Chem.*, 47, 12, (2009), 1031-1035.

[6] Zalaru, C.; Dumitrascu, F.; Draghici, C.; Tarcomnicu, I.; Marinescu, M.; Nitulescu, G.M.; Tatia, R.; Moldovan, L.; Popa, M.; Chifiriuc, M.C. New Pyrazolo-Benzimidazole Mannich Bases with Antimicrobial and Antibiofilm Activities, *Antibiotics*, 11, (2022), 1094.

[7] Marinescu, M.; Popa, C.V.; Tănase, M.A.; Soare, A.C.; Tablet, C.; Bala, D.; Cinteza, L.O.; Dițu, L.M.; Gifu, I.C.; Petcu, C. 2022, 15, 8162. Synthesis, Characterization, DFT Study and Antifungal Activities of Some Novel 2-(Phenyldiazenyl)phenol Based Azo Dyes. *Materials*, 15 (2022), 8162.

SC-P07 ELECTRODEPOSITION OF AMORPHOUS NICKEL / GOLD LAYER(S) AND ALLOYS ON A COPPER SUBSTRATE FOR ELECTRICAL CONNECTORS

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Abstract: *The rapid development of the electronics industry makes it essential to design efficient methods for better electrical connectors. Traditionally, they are coated by noble metals characterized by high electrical conductivity. The strategy investigated in this study is aimed at copper contacts electroplated with gold and nickel separate layers or their co-deposition from environmentally friendly, cyanide-free baths. Also, the present work aims to achieve a trade-off between electrodeposition time and thickness of the deposited layer, an important aspect for the transposition of the strategy to industrial scale. The characteristics of the deposited layer were investigated from a morphological and compositional point of view, using scanning electron microscopy, but also from a functional point of view, by measuring the resistivity, using the four-probe method.*

Key words: electroplating, amorphous gold / nickel, alloy, resistivity

Introduction: Modern life cannot be imagined without electronic devices that allow us to perform tasks that were impossible even to envision in the past. To enhance their electrical conductivity, they are electroplated with platinic metals. Nickel-plated contact surfaces provide both electrical dependability and corrosion resistance [1, 2]. In this study are investigated both the electroplating with gold and nickel separate layers and also a co-electrodeposition process that uses an eco-friendly solution for an economical technology on a copper substrate.

Experimental: Gold / Nickel coatings (Au / Ni) were applied by electrodeposition or co-deposition on copper substrate from different electrolytic baths, using similar operating conditions. In order to determine the optimal conditions for Ni and Au electrodeposition, morphological characterization of the deposited Au-Ni coatings was performed by SEM, and the functionality was evaluated by measuring the electric resistivity, using the four-probe method [3]. After preliminary treatment of the copper samples, two sample sets were prepared, one using the one at a time deposition approach and the other the co-deposition of the gold / nickel alloy. The electroplating cell consisted of two electrodes: platinum as the insoluble anode and a pure cooper sheet as the cathode. DC or pulsed current plating techniques were utilized (VoltaLab 40 potentiostat), with average current densities of 1.8–6.0 mA/cm^2. Different molar ratios for $NiCl_2 \cdot 6H_2O$: $KAuCl_4$ were tested for Au-Ni plating. The solutions studied in this work have the following composition: tri-

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ammonium citrate 0.411 mol/L, potassium gold-chloride 0.066 mol/L, sodium sulphite 0.563 mol/L and variable quantities of nickel chloride hexahydrate.

Results and discussions: The addition of nickel chloride does not deteriorate the pure gold solution, although the solution colour is changed from faint yellow to green. In fact, the plating rate for Au-Ni films is still about 10 µm per hour, which is similar to the rate for pure gold from a gold plating solution. The deposited film is smooth if plated at 4.0 mA/cm^2 and becomes rough if plated at greater current densities. This observation implies that the addition of nickel chloride does not change significantly the plating process.

Table 1. Experimental results of Ni and Au electrodeposition on copper substrate samples

No.	**Samples**	**m_{Ni} (g)**	**m_{Au} (g)**	**d_{Ni} (µm)**	**d_{Au} (µm)**	**R bulk (mΩ)**	**R surface (mΩ)**
1.	X"	0.0109	0.0074	12.2472	3.8342	0.10	0.129
2.	Y"	0.0110	0.0117	12.3596	6.0622	0.11	0.094
3.	Z"	0.0102	–	11.4607	–	0.08	0.158
4.	Cu	–	–	–	–	0.05	0.208

Conclusions: The pulse plating process has the advantage of producing finer grain deposits than the DC process. This fact is due to the high current density value that produces a high nucleation rate, which also leads to low porosity. Films plated at a current density of 4.0 mA/cm^2 have nickel concentrations of 0.8 – 1.3 %. Increasing the nickel chloride concentration in the electroplating solutions has two side effects on the plating process: increases the nickel concentration in the plated films, which is desirable for hard gold plating, and also increases stress in the electrodeposited films, that induces. However, from the electrical resistance measurements, it can be seen that a greater thickness of deposited nickel and gold layers has a direct proportional influence on the efficiency of the electrical contact, both for bulk or surface resistivity.

References:

[1] Y. Nishimura, M. Maebara, K. Tashiro, H. Honma, T. Yamashita, “Surface Morphology and Characteristics of Electroplated Au/Ni Films for Connector Contact Materials”, *Transactions of The Japan Institute of Electronics Packaging*, vol. 6, no. 1, pp. 18-23, 2013

[2] A. He, Q. Liu, D. G. Ivey, “Electroplating of Gold from a Solution Containing Tri-ammonium Citrate and Sodium Sulphite”, *Journal of Material Science: Material Electronics*, vol. 20, pp. 543-550, 2009

[3] A. He, Q. Liu, D. G. Ivey, “Electroplating of Au-Ni and Au-Co Alloy Films”, *Plating & Surface Finishing*, vol. 96, no. 5, pp. 22-29, 2009

[4] E. C. Estrine,a S. Riemer,b V. Venkatasamy,b B. J. H. Stadler,a and I. Tabakovica, “Mechanism and Stability Study of Gold Electrodeposition from Thiosulfate-Sulfite Solution”, *Journal of The Electrochemical Society*, vol. 161, no. 12, pp. D687-D696, 2014

SC-P08 EVALUATION AND MODELING OF A Li-ION BATTERY AT VARIOUS DISCHARGE RATES

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Abstract: *Lithium-ion (Li-ion) batteries have emerged in the last three decades as an important energy storage device, providing high capacity, high energy density and long-term reliability for various applications. Moreover, due to increase demands of different electric devices of various sizes and shapes, electric vehicles included, they tend to become more and more as the favorite portable power sources. One of the drawback when using such devices is that the performance of Li-ion batteries deteriorates with increasing number of charge/discharge cycles and the fact that the state of charge at any given moment is not easily predictable, only the energy consumption is accounted for by the method of coulomb counting. In this paper we present how one may determine experimentally the actual battery capacity and its internal resistance for an 18650 Li-Ion battery type and we propose a first degree model for determining the state of charge (SoC) (which indicates the remaining battery capacity at any given time, strongly related to operating autonomy of the considered device) as well as the state of health (SoH, battery aging) and the maximum operating time at maximum current yield.*

Such information may be particularly useful to prevent batteries from becoming over-charged or over-discharged, to predict the driving range of electric vehicles etc.

Key words: Li-ion battery, capacity, internal resistance, discharge modeling, state of charge

References:

[1] Saxena, V., Sharma, A., Kothari, R., Sahu, S. K., & Kundalwal, S. I., Analysis of Li-ion battery under high discharge rate embedded with metal foam phase change composite: A numerical study. *Journal of Energy Storage*, *84,* (2024). 110752.

[2] Özdemir, T., Ekici, Ö., & Köksal, M. (2024). Numerical and experimental investigation of the electrical and thermal behaviors of the Li-ion batteries under normal and abuse operating conditions. *Journal of Energy Storage*, *77*, 109880.

[3] Lijesh, K. P., & Khonsari, M. M. (2024). A thermodynamic approach for characterizing the degradation of Li-ion batteries. *Journal of Energy Storage*, *82*, 110565.

[4] Chen, X., Hua, W., Yuan, L., Ji, S., Wang, S., & Yan, S. (2023). Evolution fate of battery chemistry during efficient discharging processing of spent lithium-ion batteries. Waste Management, 170, 278-286.

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SC-P09 SYNTHESIS AND CHARACTERIZATION OF NEW PYRAZOLE COMPOUNDS WITH ANTIBACTERIAL ACTIVITIY

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Abstract: *New pyrazole derivatives with antibacterial properties were synthesized and characterized by spectroscopic methods*

Key words: pyrazoles, NMR, IR, UV-Vis, bacterial strains

Introduction: The pyrazole nucleus is receiving considerable attention due to the diversity of its therapeutic properties [1]. The development of new antimicrobial drugs involves the identification of innovative antimicrobial agents, among which are pyrazole derivatives [2]. A series of pyrazole derivatives were synthesized and characterized physico-chemically by IR, NMR, UV-Vis spectroscopic methods, as well as tested for their antibacterial activity [3-5].

Experimental: All reagents were purchased from Merck Millipore. Intermediate pyrazole compounds were synthesized, characterized and tested on bacterial strains. A series of pyrazole, pyrazolo-benzimidazole, azopyrazole derivatives was obtained, characterized from a physico-chemical point of view and tested on Gram-Positive, Gram-Negative bacterial strains, to highlight the antibacterial activity.

Results and discussions: The synthesis of pyrazole derivatives and its hybrids, Mannich bases was carried out in two steps, the compounds obtained, good reaction yields. Azopyrazoles were obtained by diazotization-coupling reactions. All the compounds demonstrated very good antibacterial activity on the bacterial strains tested in comparison with the reference drugs.

Conclusions: A series of pyrazolicines and pyrazolo-benzimidazoles, azopyrazoles derivatives were synthesized, characterized by spectroscopic methods, by confirming the proposed structure and tested on bacterial strains. A correlation of their structure with antibacterial activity could be explained.

References:

[1] El-Gohary N.S., Shaaban M.I., Synthesis, antimicrobial, antiquorum-sensing and antitumor activities of new benzimidazole analogs, *Eur. J. Med. Chem.* 137 (2017) 439-449.

[2]. Sharma P.K., Chandak N., Kumar P., Sharma C., Aneja K.R., Synthesis and biological evaluation of some 4-functionalized-pyrazoles as antimicrobial agents, *Eur. J. Med. Chem.* 2011, *46(4),* 1425-1432.

[3]. Zalaru, Ch., Dumitrascu F., Draghici C., Tarcomnicu I., Tatia R., Moldovan L.,. Chifiriuc M.C, Lazar V., Marinescu M., Nitulescu M.G., Ferbinteanu M., Synthesis, spectroscopic characterization, DFT study and antimicrobial activity of novel alkylaminopyrazole derivatives. J. Mol. Struct. 1156 (2018) 12-21.

[4]. Marinescu M., Tudorache D.G., Marton G., Zalaru C., Popa M., Chifiriuc C.M., Constantinescu C., Synthesis, DFT study and antimicrobial features of some benzimidazole derivatives, Journal of Molecular Structure 1130 (2017) 463-471.

[5] Zalaru Ch. , Dumitrascu F., Draghici C., Tarcomnicu I., Marinescu M., Nitulescu G.M., Tatia R., Moldovan L., Popa M., Chifiriuc M.C., New Pyrazolo-Benzimidazole Mannich Bases with Antimicrobial and Antibiofilm Activities. *Antibiotics*, 2022, 11 (8), 1094.

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SC-P10 MERWINITE BASED BIOCERAMIC SCAFFOLDS PROCESSED VIA ROBOCASTING

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Abstract: *Merwinite based powders were synthesized using two approaches and were characterized using X-ray diffraction. Those powders were successfully processed to obtain 3D structures with potential in bone replacement using the robocasting technique.*

Key words: Merwinite, 3D printing, robocasting, bone scaffolds

Introduction: Bone tissue engineering came to be in the recent years one of the main attractions in medical research filed due to the fact that hard tissue is the second most transplanted tissue at a global level. The high demand of bone transplants is caused by numerous accidents, pathologies, and prolonged lifetime span and consequently the medical industry requires adequate bone substituents [1]. Using bioceramics from the system CaO-MgO-SiO2 (ex. Merwinite) and highly controllable processing technique like robocasting, a grafting material with tremendous potential in bone replacement could be obtained [2,3].

Experimental and/or Modelling: Merwinite based powders were synthetized using two different approaches: sol-gel synthesis and combustion synthesis. The obtained powders were characterized using X-Ray diffraction (XRD). Furthermore, the synthesized materials were processed using a 3D printing technique called robocasting. Several ratios between powder and additives were tested to obtain a paste with suitable rheology. Scaffold of 20x20x3 mm, a strand thickness of 0.6/ 0.8 mm, with infill of 20-25%, rotation angle between layers of 90°, and linear pattern were obtained. The 3D structures were characterized using Scanning Electron Microscopy (SEM).

Results and discussions: Merwinite based powers were obtained using both sol-gel and combustion approaches. XRD testing indicates that both synthesis method led to powders with more than one phase, with Merwinite being one of the main identified phases**.** The obtained powders were further processed via robocasting. The results indicate that the powders obtained by both synthesis method presented adequate characteristics for the 3D printing process (Fig. 1a). Both powders required the same additive to obtain a homogenous paste, but they present different requirements when it comes to the ratio between the powder and additive. The powder synthesized by sol-gel required far less additive in order to obtain a printable paste compared to the power obtained by combustion method. The 3D

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structures were characterized using SEM (Fig. 1b and c) and it was determined that the quality of the strands was good and that the printing parameters were respected.

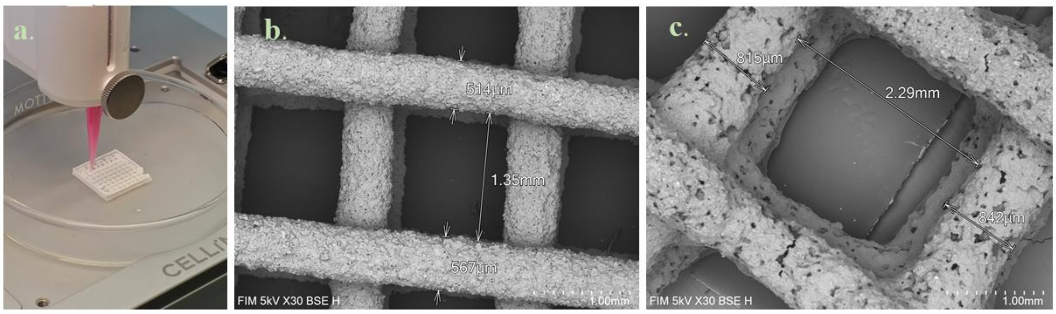

Fig. 1 (a) Merwinite based 3D structure obtained via robocasting process, (b) SEM image of 3D structure obtained using merwinite synthesized by sol gel, (c) SEM image of 3D structure obtained using merwinite synthesized by combustion.

Conclusions: Merwinite based powders were synthesized using two different approaches. The 3D printing process was conducted successfully for both powders and the influence of the synthesis method to powder to additive ratio was identified. Furter investigations regarding the mechanical and biological properties is required in order to assess the prospect of those scaffolds in bone tissue engineering, but the robocasting potential of merwinite based powders was demonstrated so far.

References:

[1] Oryan A, Alidadi S, Moshiri A, Maffulli N. *Bone regenerative medicine: classic options, novel strategies, and future directions, J Orthop Surg* Res., (2014)

[2] Collin M.S., Venkatraman S.K., Sriramulu M., Shanmugam S., Drweesh E.A., Elnagar M.M, Mosa E.S., Sasikumar S., *Solution combustion synthesis of functional diopside, akermanite, and merwinite bioceramics: Excellent biomineralization, mechanical strength, and antibacterial ability, Materials Today Communications*, (2021)

[3] Collins M. N., Ren G., Young K., Pina S., Reis R. L., Oliveira J. M., *Scaffold Fabrication Technologies and Structure/Function Properties in Bone Tissue Engineering. Advanced Functional Materials*, (2021)

SC-P11 ELECTOCHEMICAL SYNTHESIS OF TiO_2 AND Ag-TiO2 NANOPARTICLES USING NOVEL DEEP EUTECTIC SOLVENT FORMULATIONS

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Abstract: *The research presents some experimental results regarding the electrochemical synthesis and characterization of TiO_2 and Ag-TiO_2 nanoparticles involving choline chloride based ionic liquids. The nanoparticles were analyzed using Scanning Electron Microscopy and X-Ray Diffraction*

Key words: nanoparticle's synthesis, deep eutectic solvents, electrochemical synthesis, antimicrobial and photodegradation properties, biomedical field.

Introduction: TiO_2 and Ag-TiO_2 nanoparticles (NPs) are used in the biomedical field due to the antimicrobial and photodegradation properties. The electrochemical route represents a simple and cost-effective procedure to synthesize these NPs. A promising alternative of aqueous electrolytes during electrochemical synthesis is represented by deep eutectic solvents (DESs), which are environmentally friendly, cost effective and exhibit stability concerning air and moisture [1][2].

Experimental: TiO_2 NPs were obtained through anodic dissolution of Ti metal in deep eutectic solvents formulations based on the mixture of choline chlorine: ethylene glycol (1:2 molar ratio). The synthesis was performed at a constant current density of 40 mA/ cm^2 for 3 h. The electrolyte containing TiO_2 NPs was subjected to cleaning by centrifugation using water and ethanol. Furthermore, the sample was dried (100 °C, 1 h) and calcined (600 °C, 2 h). Ag NPs have been electrochemically deposited on the TiO_2 NPs involving the "sacrificial anode" method using the same DES electrolyte. Different pulsed plating parameters were investigated, and the electrodeposition time varied from 1 h up to 6 h. The result mixture containing Ag-TiO_2 NPs was subjected to the same washing protocol.

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Results and discussion: TiO_2 and Ag-TiO_2 NPs were analyzed using Scanning Electron Microscopy (SEM) and X-Ray Diffraction (XRD). According to the SEM images, it was found that the obtained TiO_2 NPs have sizes between 10 and 20 nm. XRD confirmed the obtaining of the anatase phase with an average crystallite size of 14.4 nm. For the Ag-TiO2 NPs, XRD also confirms the presence of Ag when the synthesis was performed at longer times, such as 4 h or 6 h. When the process was fixed to only 1 h, the peaks assigned to Ag cannot be distinguished on the diffractogram. Complementary analysis such as Energy-dispersive spectroscopy (EDS) can show the presence of Ag even after one hour of electrochemical synthesis.

Conclusion: A new electrochemical method of synthesis was developed using deep eutectic solvents. This method can increase applications area of the NPs.

Acknowledgements: This project has received funding from GNAC ARUT 2023 project, NANO_NP_DES, entitled "Electrochemical synthesis of hybrid nanoparticles Ag/TiO_2 and Ag/Fe_3O_4 with biomedical applications".

References:

[1] A. Petica, A. Florea, C. Gaidau, D. Balan, and L. Anicai, "Synthesis and characterization of silver-titania nanocomposites prepared by electrochemical method with enhanced photocatalytic characteristics, antifungal and antimicrobial activity," *J. Mater. Res. Technol.*, vol. 8, no. 1, pp. 41–53, 2019, doi: 10.1016/j.jmrt.2017.09.009.

[2] A.P. Abbott, G. Frisch, K.S. Ryder, Electroplating using ionic liquids, Annu Rev Mater Res 43 (2013) 335–358. https://doi.org/10.1146/annurev-matsci-071312-121640.

BOOK OF ABSTRACTS

SICHEM – 2024

D – Green applied chemistry and agro-resources valorization (GACARV)

1. Keynotes

SD-KN01 POLYPHENOLIC EXTRACTS FROM VARIOUS RAW-MATERIALS. BENEFICIAL PROPERTIES PRESERVATION THROUGH INCORPORATION IN MESOPOROUS SILICA-TYPE SUPPORTS

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Abstract: *In this study was analyzed the chemical profile of several polyphenolic extracts prepared using different raw-materials, solvents and extraction techniques. The biological characteristics of chosen extracts free and embedded in mesoporous silica-type supports were also assessed as well as extracts stability in time.*

Key words: berries, extraction techniques, polyphenols extracts, chemical profile, embedded extracts

Introduction: Polyphenolic extracts from different vegetal materials present high amounts of antioxidants, antimicrobials, having antidiabetic or antitumor effects [1,2], but they are prone to a faster degradation [3]. The embedding of extracts in different silica-type supports, with high porosity, allows the improvement of extracts stability in time. The purpose of this study was to evaluate differences on chemical profile depending on type of vegetal material and extraction conditions, both influenced the characteristics of extracts free or incorporated in mesoporous silica-type supports.

Experimental: The chemical profile of prepared extracts was assessed through HPLC-PDA and spectrophotometric methods (polyphenols, flavonoids and anthocyanins). The radical scavenger activity of embedded extracts was compared to that of the free extract and support. The supports and materials containing extract were also analyzed by FT-IR spectroscopy, N_2 adsorption-desorption isotherms and thermal analyses. The biological effects of embedded extracts were carried out and compared with that of the free extract.

Results and disscusions: The extracts from different wild berries had high amounts of polyphenols, in the range of 35.11-177.04 mg gallic acid equivalent/g extract, the highest values being obtained for cranberry extracts. All extracts prepared from wild berries presented good radical scavenger activity, in the domain of 26.90-187.76 mg Trolox equivalent/g extract. An investigation regarding whether extraction parameters influence the amount of recovered beneficial compounds was performed. For the incorporated extracts in silica-type supports, enhanced

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antioxidant potential was noticed, when compared to the free extract, after various storage times, in dark conditions, at 4 °C, which could be explained by a faster degradation of the free extracts.

Conclusions: Extract-loaded mesoporous silica-type supports exerted longer chemical or thermal stability than the corresponding free extract. Having good antioxidant, antimicrobial or anti-inflammatory properties, they could be used for producing nutraceutical or cosmetic products.

Acknowledgements: This work was supported by a grant of the Romanian Ministry of Education and Research, PCE 117/2022 COMCONF.

References:

[1] Buda V. *et al.*, Biological Evaluation of Black Chokeberry Extract Free and Embedded in Two Mesoporous Silica-Type Matrices. *Pharmaceutics* 12 (2020), 838.

[2] Brezoiu A.-M., Deaconu M., Mitran R.-A., Sedky N.K., Schiets F., Marote P., Voicu I.-S., Matei C., Ziko L., Berger D. The Antioxidant and Anti-Inflammatory Properties of Wild Bilberry Fruit Extracts Embedded in Mesoporous Silica-Type Supports: A Stability Study. *Antioxidants*, 13, (2024), 250.

[3] Antony A., Farid M., Effect of Temperatures on Polyphenols during Extraction. *Applied Sciences*. 12(4), (2022), 2107.

SD-KN02 IMPROVEMENT OF METABOLIC DISORDERS WITH THE HELP OF GEMMOTHERAPY

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Abstract: *Gemmotherapy, also known as plant bud therapy or embryonic phytotherapy, is a form of herbal medicine that uses extracts from the buds, young shoots, and rootlets of various trees and shrubs. For metabolic disorders we use a gemmotherapic treatment plan that contains: diluted glycerinohydroalcoholic extract 1 DH from Acer campestre buds,Ribes nigrum buds,Cornus sanguinea buds,Hordeum vulgare fresh roots, Fraxinus excelsior buds, Corylus avellane buds. Glycerinohydroalcoholic extracts can be administered in combination with other therapies, either allopathic or natural, without interfering with their action.*

Key words: metabolic diseases,gemmotherapy,buds

Introduction: Metabolic diseases encompass a broad range of disorders that affect the body's ability to process nutrients and energy. While some metabolic diseases are genetic and present from birth, others may develop later in life due to environmental factors or lifestyle choices. Here's a brief overview of some well-known metabolic diseases: phenylketonuria, homocystinuria, nonketotic hyperglycinemia,galactosemia, fructose intolerance,familial hypercholesterolemia, type 2 diabetes, hemochromatosis, porphyria,gout,obesity[1].

Experimental: Gemmotherapy, also known as plant bud therapy or embryonic phytotherapy, is a form of herbal medicine that uses extracts from the buds, young shoots, and rootlets of various trees and shrubs. For metabolic diseases we use a gemmotherapic treatment plan that contains: diluted glycerinohydroalcoholic extract 1 DH from *Acer campestre* buds,*Ribes nigrum* buds,*Cornus sanguinea* buds,*Hordeum vulgare* fresh roots, *Fraxinus excelsior* buds, *Corylus avellane* buds[2,3].

Results and discussions : The study was carried out on a group of 20 patients aged between 20-80 years who has a wide range of metabolic diseases.Administration of glycerinohydroalcoholic extracts for 6 months to patients who presented themselves in the apiphytotherapy office was considered.

Conclusions: Over the years, gemotherapy has proven effective in many types of both acute and chronic conditions.Glycerinohydroalcoholic extracts can be administered in combination with other therapies, either allopathic or natural, without interfering with their action.

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References:

[1] Daniel J. Hoffman, Theresa L. Powell,Emily S. Barrett, Daniel B. Hardy, Developmental origins of metabolic diseases, *American Physiological Society,* 0031-9333,ISSN1522-1210, 739 – 795,2021

[2]Anca Daniela Raiciu,*Aplicatii farmacognostice si gemoterapice*,partea I, Editura Universităţii „Titu Maiorescu, Editura Hamangiu,ISBN 978-606-767-071-4,2020

[3]Anca Daniela Raiciu,*Aplicatii farmacognostice si gemoterapice*,partea II, Editura Universităţii „Titu Maiorescu, Editura Hamangiu,ISBN 978-606-27-1604-2,2020

BOOK OF ABSTRACTS

SICHEM – 2024

D – Green applied chemistry and agro-resources valorization (GACARV)

2. Oral presentations

SD-OP01 EVALUATION OF RESEARCH INTERESTS FOR MICROPLASTICS IN ROMANIA

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Abstract: *Global research was and is the engine behind the development of the economy and not least the creation of new jobs in various sectors, while at the same time having a major influence in all other spheres of development such as trade, environment, education, and health. At the European level, this research-development component is a major point of interest in development strategies. In Romania, research is carried out in higher education institutions as well as in national research institutes with the role of developing Science and Technology to increase the competitiveness of the Romanian economy and increase knowledge with the potential for capitalization and widening the horizon of action. This study shows that research on plastic/microplastic pollution (MPS) is at a low level, even insufficiently studied in Romania, where there are still deficiencies in household waste management. The knowledge gaps identified so far suggest new research directions in the area of MPS which is at a pioneering level in Romania, plastic studies, and MPS being identified in a few Institutes and Universities in Romania, through this study. At the global level, the abundance of MPS has been studied more intensively in recent years in marine and freshwater environments, and in other environments, in Romania, it is completely absent. The increase in plastic production and the large-scale use of plastic materials results in the accumulation of large amounts of plastic waste in the environment, being a global challenge that must be addressed because the natural aging process of macroplastics generates a multitude of secondary microplastic fragments that accumulates in all areas of the planet. According to the Science and Research Barometer - the State of the Nation project, (2018) Romanians attach importance to the field of Science and Technology, but at the same time, it does not have a counterpart in the importance given over time by the governments of Romania. The funding granted to this field is below one percent of GDP, which puts us at the bottom of the European ranking, compared to the states in the region (Hungary, Poland, Bulgaria), and the long-term impact of the underfunding of the research field in Romania is negative and difficult to estimate (National Institute of Statistics, 2024).*

Keywords: Microplastic particles, Research interests, Research gaps, Romania;

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SD-OP02 NAVIGATING WATER VULNERABILITIES IN RURAL SETTINGS: INVESTIGATING THE IMPACT OF AGRICULTURAL ACTIVITIES ON DRINKING WATER QUALITY

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Abstract: *In agricultural settings, drinking water resources are susceptible to contamination and pollution from various sources, such as runoff from fields, leaching of fertilizers and pesticides and soil erosion among others. Understanding the impact caused by these agricultural activities on water quality is essential for ensuring safe drinking water to rural communities. This research explores the evaluation of water quality characteristics in areas where agriculture is practiced, Mihaileni village, concentrating on pH, salinity, turbidity, Electrical Conductivity (EC), Oxidation-Reduction Potential (ORP), and Total Dissolved Solids (TDS). Through the examination of these factors in water samples gathered from diverse sources (wells), the research seeks to offer insight on the possible impact of agricultural activities on drinking water supplies. A thorough campaign of sampling was carried out at several locations in the research region in order to gather water samples for examination. Using common analytical methods, parameters including pH, ORP, EC, TDS, salinity, and turbidity were assessed. The outcomes were then evaluated for compliance and departures from permissible limits by comparing them to established water quality criteria. The investigation's conclusions showed that, generally, the measured salinity, pH, ORP, EC, and TDS in the collected water samples fell within permissible bounds in accordance with legal requirements for drinking water quality. Nonetheless, there were noticeable differences in the turbidity levels, with certain samples having more turbidity than others. The elevated turbidity levels observed in certain samples indicate a potential concern for water quality in agricultural areas. Turbidity, often attributed to suspended particles such as soil, sediment, and organic matter, can impact the aesthetic quality of water and may serve as a carrier for pathogens and other contaminants. The presence of higher turbidity in specific samples suggests a potential link to agricultural activities, such as soil erosion, runoff from fields, or inadequate management practices. In conclusion, while most water quality parameters remained within acceptable ranges, the presence of higher turbidity in certain samples indicates a potential risk to drinking water resources in agricultural areas. Further research and monitoring efforts are warranted to better understand the sources and implications of elevated turbidity and to implement effective management practices to ensure the provision of safe and reliable drinking water to communities.*

Keywords: water quality, agricultural impact, rural communities

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SD-OP03 GLYCEROL CONVERSION TO LACTIC ACID: PROCESS ANALYSIS

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Abstract: *In this work, a conceptual design of lactic acid process synthesis from glycerol was carried out. The mass and thermal balance, together with the sizing of the main equipment were necessary for the proposed process calculations, which showed economic feasibility.*

Key words: Glycerol valorization, lactic acid, process modeling, economic evaluation

Introduction: Lactic acid is a well-known α-hydroxy-monocarboxylic acid presenting various applications. In the food industry it is mostly used for pH adjustments, as flavoring agent, or preservative, in the cosmetics it is applied in cuticle removal solutions or anti-acne treatments, while in the polymer industry, is the main raw material for obtaining polylactic acid, a biodegradable polymer. A recent pathway to produce lactic acid is using glycerol as raw material, a biodiesel byproduct, instead of the chemical route which could involve the toxic lactonitrile [1].

Modelling: In the proposed process, lactic acid is being produced through glycerol chemical conversion in a continuous reactor, in the presence of a copper catalyst. The chemical plant production capacity was 30000 tonne/yr of 80 % wt. lactic acid solution. A process flowsheet was developed, and the mass and heat balance calculations have been performed, either through balance equations or using Aspen Plus v10 commercial simulator.

Results and discussions: The process flowsheet could be divided into three sections, a reaction one in which glycerin is converted to sodium lactate, a lactic acid purification and recovery section, and a third one for the byproducts separation. Besides lactic acid, other important products including propylene glycol and diglycerol are obtained with high purity and are further valorized [1]. To evaluate economically the proposed process, the main equipment characteristics were evaluated, and a sizing was performed for the multitubular heat exchanger that preheats the glycerol solution.

Conclusions: An economic feasibility of the proposed process was achieved considering that the determined production price of 1.64 $/kg being relatively lower than lactic acid market price of 1.9 $/kg.

References:

[1] Zavrazhnov S., Esipovich A., Zlobin S., Belousov A., Vorotyntsev A. Mechanism Analysis and Kinetic Modelling of Cu NPs Catalysed Glycerol Conversion into Lactic Acid, Catalysts, 9(3), (2019), 231.

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SD-OP04 ASSESSMENT OF HEAVY METAL CONTAMINATION ON AGRICULTURAL SOILS IN THE VICINITY OF A HISTORICALLY POLLUTED AREA IN TURDA, CLUJ COUNTY

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Abstract: *Heavy metal contaminated soils in Romania have gained the attention of experts, due to the recent environmental regulations set for contaminated sites. To evaluate such an area in Turda (Cluj county), a chemical assessment was conducted in the proximity of a former chemical plant. The total metal content was determined in various soil samples collected from the study site. The analyses were performed with flame atomic absorption spectrometry. To evaluate the potential environmental risk, the bioavailable fraction was also analyzed to be correlated with possible plant uptake. Principles of the sequential extraction technique were considered for the evaluation of the mobile forms of heavy metals. The results were confronted with the Romanian environmental legislation and increased metal contamination was observed in the analyzed soil samples. At the same time, a potential level of soil contamination with bioavailable forms of heavy metals (in particular Cu, Zn, Cd) was indicated by the chemical assessment.*

Keywords: soil, contamination, heavy metals, historical pollution, bioavailable fraction, risk.

Introduction: In Romania, there are various sources of heavy metal contamination, mainly from anthropogenic activities. Results from studies over the last ten years show that soil is significantly affected by this type of pollution[1]. The investigation was conducted to assess the impact of heavy metal contamination on agricultural lands near the former chemical plant. The aim of the research is to determine the potential for contamination and bioaccumulation of heavy metals in soil associated with industrial activity. To evaluate potential risks to human health, ecosystem health, and food safety, a sequential analysis of the total and bioavailable fractions of heavy metals in soil was deemed necessary.

Experimental and/or Modelling: The selection of soil sampling points was carried out in accordance with Annex 3 of the Romanian Order No. 184/1997. For the determination of physico-chemical parameters, a 1:5 aqueous extract (soil-distilled water) was used, followed by agitation, settling, and filtration. The measurements were performed by using the WTW-multi 350i multiparameter device. Moisture content was determined by drying the samples in an oven at 105°C for 24 hours. For the determination of heavy metals, the samples were dried in an oven, ground, sieved, weighed, mineralized with *aqua regia* ($HCl:HNO_3$ 3:1) for 8 hours, and heated on a sand bath for 2 hours. Analysis was performed using flame atomic absorption spectrometry (AAS-F) with the assistance of the AAS ZEEnit 700 Analytik Jena instrument. To determine the bioavailable fraction (SR ISO 14870:2001), a method of extracting oligoelements from soil samples using a

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diethylenetriaminepentaacetic acid (DTPA) buffer solution was used. The assessment of the degree of heavy metal soil contamination was performed using specific factors.

Results and discussions: Following the investigations regarding the contamination of agricultural lands in the industrial area of Turda municipality, the results highlight a potential level of soil contamination with bioaccumulative heavy metals (in particular Cu, Zn, Cd) in the studied area, as a result of historical pollution generated by past industrial activities. According to the obtained data, a significant level of bioaccumulation is highlighted in certain soil samples for Cu, Cr, Zn, and Cd.

Conclusions: This finding carries important implications for the decision-making process of authorities regarding soil management, remediation, and risk assessment. It can be assumed that conducting detailed investigations in the industrial area of Turda city, with particular emphasis on the zones near the former chemical plant, is crucial to determine the extent and impact of heavy metal contamination. By implementing sustainable strategies, it is possible to protect both human health and the integrity of the environment against the adverse effects of this form of contamination. It is necessary to develop a monitoring system for these areas, as well as a method for a more precise assessment of the effects of these metals on human health[2].

References:

[1] Iosob, G.A., Bute, A., Calara, M., Antal-Tremurici, A., Benchea, C.M., Bouruc, D., Avasiloaiei, D.I., Muscalu, S.P. (2020). Heavy metals contamination of soil and vegetables in three regions from Romania: A review, Studies and Research, "Vasile Alecsandri" University of Bacău;

[2] Brișan, N., Roba, C., Bălc, R., Ulinici, S., Oltean, V.I., Boar, F. (2022), Heavy metals concentration in different species of trees, shrubs and the associated soils from urban area of Cluj-Napoca, România, In: Ecological and environmental chemistry: 2022, Ed. 7, 3-4 martie 2022, Chișinău, Republica Moldova, Centrul Editorial-Poligrafic al USM, 2022, Ediția 7, Vol. 2;

SD-OP05 OBTAINING CELLULOSE MEMBRANES EXTRACTED FROM *ULVA LACTUCA* ALGAE

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Abstract: *In this study, the extraction of cellulose nanofibers from Ulva Lactuca was performed by precipitation with ethanol.*

Key words: *Ulva Lactuca*, membranes, cellulose.

Introduction: Algae are a sustainable source for the global demand of biopolymers without affecting food supply. Biopolymers obtained from algae seem to have great perspectives due to their high photosynthetic efficiency.

Experimental: Fresh *Ulva Lactuca* algae was harvested from the north of the Romanian Black Sea Coast. The extraction of cellulose from *Ulva Lactuca species* was performed in a water bath with weak magnetic agitation. Then, the following substances were added in different concentrations: sodium hydroxide, ammonium oxalate, acetic acid and hydrochloric acid for bleaching. To obtain the extracted cellulose membranes: in a alkaline solution of sodium hydroxide and thiourea, the cellulose powder was added under controlled agitation. Then the solution was cooled at -10°C. After that the cellulose gel was washed with a slow acid solution with formaldehyde. Then they were washed with distilled water until neutral pH.

Results and discussions: The dry cellulose extracted from algae were subjected to observation by transmission under the SEM TM4000 Tabletop SEM microscope (Hitachi, Japan). In order to highlight the functional groups of species in the *Ulva Lactuca* algae sample, the equipment for FTIR -Tensor 37 Bruker analyses (Woodstock, NY, USA) was used.

Conclusions: The highest yield, 20,944 % of extracted cellulose per dry matter was obtained for the following factors: S/L=1/20; conc. ethanol=90%, conc. salts=4 g/L. The swelling of biocellulose membranes in alcoholic solutions of high concentrations was investigated. The low swelling in concentrated ethanol indicates that it is possible to use these membranes for ethanol dehydration of ethanol solutions with a composition similar to the ethanol/water azeotrope.

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SD-OP06 SUPERIOR VALORIZATION OF FORGOTTEN BERRIES - *PRUNUS SPINOSA* L. (BLACKTHORN)

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Abstract: *This study aimed at establishing the effects of extraction process factors on the composition and antioxidant activity of Prunus spinosa L. (blackthorn) fruit extracts.*

Key words: *Prunus spinosa* L.; antioxidant capacity; phenolic compounds; optimization.

Introduction: Blackthorn fruits contain different polyphenolic compounds, *e.g.*, phenolic acids, flavonoids, anthocyanins, coumarins, which determine their antioxidant, antimicrobial, anti-inflammatory, and anticancer properties [1].

Experimental and modeling: Fruit lipids were removed by extraction with isooctane for 2 h at room temperature. The mixture was filtered, and the solid phase was dried prior to its use for the extraction of polyphenolic compounds. Mixtures of ethanol and water acidified with 0.6% (*v/v*) lactic acid were used as extraction solvents. Ethanol concentration in the extraction solvent (50–100% v/v), extraction temperature (30–82.5°C), and extraction time (5–180 min) were selected as process factors. The extracts were analyzed to determine total phenolic content (*TPC*), total anthocyanin content (*TAC*), antioxidant capacity (*AC*), and chemical composition by the HPLC method. Response surface regression models were used to quantify the effects of extraction process factors on *TPC* and *TAC*.

Results and discussion: A synergistic effect of obtaining high values of *TPC*, *TAC*, *AC*, protocatechuic acid, and vanillic acid was achieved for the extraction in 50% ethanol at 60 °C for 30 min [2]. At a higher level of process temperature, the extraction of protocatechuic acid and vanillic acid was enhanced, but the flavonoids, *i.e.*, rutin hydrate and quercetin, were degraded. A lower temperature should be used to obtain a higher amount of flavonoids.

Conclusion: Optimal extraction of different types of phytocompounds requires special experimental conditions depending on their chemical and thermal stability as well as molecular mass.

References:

[1] Tiboni M.. Coppari S., Casettari L., Guescini M., Colomba M., Fraternale D., *et al.*, *Prunus spinosa* extract loaded in biomimetic nanoparticles evokes in vitro anti-inflammatory and wound healing activities, *Nanomaterials*, 11, 1, (2020), 36.

[2] 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.

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SD-OP07 ENVIRONMENTALLY FRIENDLY LUBRICATING GREASES FROM FOOD INDUSTRY WASTE OILS

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Abstract *The production of lubricating greases from vegetable oil waste, in the context of increasing sustainability concerns and efficient resource utilization, is a challenge. Using waste oils form food industry may have a significant impact on reducing environmental pollution and spearing new raw materials in the manufacturing process.*

A first study [1] focused on obtaining 100g batches of lubricating greases from vegetable oil waste, particularly from sunflower and palm oil, emulsified with 20% wt. calcium or lithium stearate as thickener and supplemented with cellulose or lignin in various proportions. The obtained products underwent characterization, including rheological studies to assess their fluid behavior, determination of consistency through penetration tests, and morphological analysis to understand their structure.

Once the samples were validated, an attempt was made to scale up the process using 500-gram samples [2]. These larger batches were also characterized through morphological study, rheological analysis, and penetration tests for freshly prepared and for "worked" greases. Additionally, the dropping points of the greases were determined, and a grease stability test was performed. Mechanical tests were conducted to determine the friction coefficient, the film thickness in a lubricated mechanism, and the wear scares diameters in the four-ball test.

The rheological analysis showed that they are visco-plastic fluids, obeying the Bingham model whose parameters were determined, and the viscosity vs. shear rate fit to power law; in all cases, the viscosity increased with additive concentration. The consistency tests (the penetration values) for "worked" greases revealed that soft greases (1 NLGI grade) were obtained, prone to be used in applications for mechanisms with moderate loading. The greases had dropping points around 100°C, and the stability tests showed a high capacity for oil separation, characteristic to soft greases. The mechanical tests gave similar or better results than commercially available soft lubricant greases.

The results indicate that scaling up don't negatively affect the characteristics of the greases, suggesting that the process is scalable and may be appliedat industrial level.

References

[1] O.V. Săpunaru, A. E. Sterpu, C. A. Vodounon, S. Osman, C. I. Koncsag, Rheology of new lubricating greases made from renewable materials, *Ovidius University Annals of Chemistry* 34 (2023), 91 - 98, DOI: 10.2478/auoc-2023-0012

[2] O.V. Săpunaru, A. E. Sterpu, C. A. Vodounon, J. Nasr, C.Duşescu-Vasile, S. Osman, C. I. Koncsag, Lubricating Greases from Fried Vegetable Oils, *Lubricants*, 12, (2024), 2900632, in press

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SD-OP08 REMOVAL OF DICLOFENAC FROM WASTEWATER USING A SUSTAINABLE APPROACH BASED ON GREEN MICROALGAE *COELASTRELLA THERMOPHILA*

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Abstract: *This work evaluated the removal of pharmaceuticals from wastewater, such as diclofenac, by biological processes using green microalgae, Coelastrella thermophila, which could be used at the same time for biomass production.*

Key words: Green Microalgae, Diclofenac removal, Biomass

Introduction: The intensive use of pharmaceuticals for human and veterinary purposes results in their continuous release into the environment [1]. One of the most frequently detected pharmaceuticals in aqueous environment is the diclofenac sodium (DFC), a non-steroidal anti-inflammatory drug, used to treat pain, dysmenorrhea, and rheumatoid arthritis [2]. Classical methods used in wastewater treatment plants are ineffective on this kind of micropollutant and in some cases can generate other emerging contaminant with higher toxicity than the initial pollutant. Microalgal bioremediation can be an alternative remediation technology powered by solar energy, effective, environmentally friendly and sustainable [3]. In this context, the freshwater green microalga *Coelastrella thermophila* isolated from an Algerian hot spring was selected to investigate the removal of DCF from wastewater.

Experimental and/or Modelling: *C. thermophila* was isolated from Algerian hot springs named “Bir Ben Osmane lac”. Batch experiments were performed to assess the DCF removal capacity of *C. thermophila* that was incubated and maintained in growth chambers (30 °C, 25 µmol photons m^{-2} s^{-1}) in a sterile BG-11 medium. Cultures were exposed to pure DCF at initial concentrations of 0 (control), 25, 50, 100, and 200 mg L^{-1} in the culture medium. The determination of biomass production and of residual, adsorbed, accumulated, and biodegraded DCF was carried out every two days. Abiotic removal was also scrutinized by adding the same amount of DFC devoid of microalgae in culture medium. Total DCF removal percentage by *C. thermophila* and their effect on algal growth, assessed by dry cell weight (DCW), optical density, cell number, biomass and lipid production, were monitored.

Results and discussions: The *microalgae C. thermophila* was first isolated, purified, identified by molecular biology tools, and finally cultivated in flasks with and without DCF.

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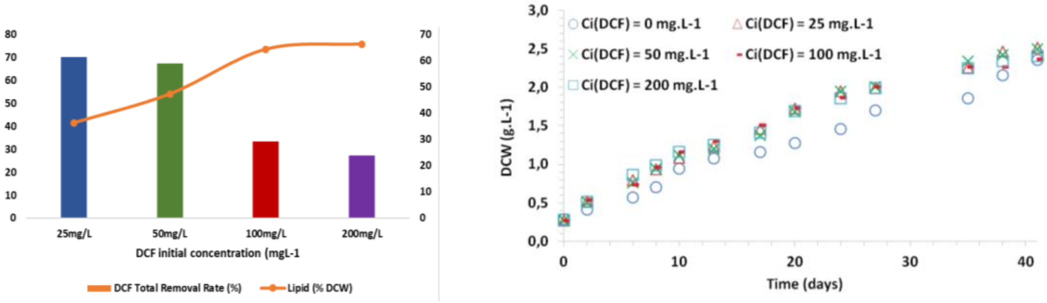
Among all the studied mechanisms, biodegradation was the major pathway for DFC elimination from water by *C. thermophila*. The biodegradation was found to be 53.5 % and 44.4 % for 25 and 50 mg L^{-1}. Figure 1a plots the DCF total removal yield and lipid production after exposing *C. thermophila* to different concentrations of DCF. This yield ranged from 70.2% to 27.3%. The effect of DCF on the growth of *C. thermophila* was evaluated by measuring DCW. The results showed that the microalgae exhibited almost the same increase in DCW with increasing DCF concentration compared to the control, indicating a slightly positive growth response (Figure 2). Thus, DCF could be used as an organic carbon source, as chlorophytes have been shown to undergo mixotrophic metabolism when media are supplemented with an organic source [3]. The biomass of *C. thermophila* also emerges as a potential source for lipid-based bioenergy production (Figure 1b) using the bioremediation process of pharmaceutical wastewater [4].



(a) **(b)**

Figure 1- (a) DCF total removal yield and lipids content in C. thermophila biomass vs the initial concentration of DCF in culture medium – (b) Effect of DCF concentration in the culture medium on the growth of C. thermophila express in dry cell weight (DCW)

Conclusions: The present study demonstrated the successful removal of DFC from aqueous media (up to 70.2%) by *C. thermophila*. The green microalgae exposed to DCF could support a sustainable approach for bioremediation of pharmaceuticals with enhanced value-added products, such as lipids, towards the production of oleochemicals.

References:

[1] Daughton C. G., Ternes T. A., Pharmaceuticals and personal care products in the environment agents of subtle change, Environ. Health Perspect. 107 (1999) 907.

[2] Munoz-Penuela M., et al., Neurotoxic, biotransformation, oxidative stress and genotoxic effects in *Astyanax altiparanae* (Teleostei, Characiformes) males exposed to environmentally relevant concentrations of diclofenac and/or caffeine. Environ. Toxicol. Pharmacol. 91 (2022) 10382.

[3] Bhatt, P., et al., Microalgae-based removal of pollutants from wastewaters: Occurrence, toxicity and circular economy. Chemosphere 306 (2022) 135576.

[4] Sharma J. et al., Metabolomic response of microalgae towards diclofenac sodium during its removal from water and concomitant recovery of pigments and lipids, Biores. Technol., 31 (2024) 19105.

SD-OP09 VALORIZATION OF *CYSTOSEIRA* SP. BROWN SEAWEED FOR THE PRODUCTION OF BIOCHEMICALS AND ENERGY

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Abstract: *This work aims at valorizing brown seaweed biomass from Moroccan Atlantic coast. Two representative species from Sidi Bouzid coast of El Jadid region Cystoseira baccata and Cystoseira mediterranea were selected for this study due to their availability and ability to produce biomolecules such as alginates, fucoïdanes, lipids, phenolic compounds, and pigments such as Fucoxanthin. The biorefinery concept was applied to achieve a sustainable valorization of these biomass and for chemicals and energy carriers such as biomethane.*

Key words: Brown seaweed, *Cystoseira* sp., Biomolecules, Alginates, Fucoidans, Biomethane.

Introduction: Seaweed biomass is recognized as an important renewable resource for bio-based processes and products, containing a wide variety of metabolites with potential applications in many fields. This biomolecular biodiversity makes algae suitable for the development of biorefinery bioprocesses, with the aim of achieving sustainable and efficient production.

Materials and methods: *Cystoseira baccata* and *Cystoseira mediterranea* were collected from Sidi Bouzid coast of El Jadida (Morocco). After harvesting, the biomass was washed and dried at 45 °C. The dried seaweeds were subjected to mechanical pretreatment to thin powder ($\leq 125\mu m$).

A variety of methods were used to extract biomolecules from algae. Sequential process allows first of all the extraction of the lipids and pigments with acetone and methanol. The depigmented powder was treated successively with HCl and Na_2CO_3 to obtain fucoidan and alginate and the evaluation of the antioxydant activity was realized [1]. Soxhlet extraction was used to recover lipids, stirred maceration with 80% methanol to extract phenolics, flavonoids and tannin, and 90 % acetone for pigments. Biomethane potential (BMP), defined as the maximum amount of methane produced from a feedstock, was also measured.

Results and discussion*:* *C. baccata* and *C. mediterranea* contain a significant number of metabolites of interest (Table 1). The contents of alginates and fucoidans are

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close to those described in literature for other species of *Cystoseira* sp., such as *C. barbata* [2]. They also chow a very important antioxidant activity using different methods. the total lipids content of the two species is close to 2% and it is higher compared to *C. sauvageauana* using Soxhlet extraction with hexane [3], phenolic, flavonoids and tannin yield depend on the species. The fucoxanthin yield of the two species is close to those described in literature for other species of *Cystoseira* sp., such as *C. indica* [4]. BMP applied to *Cystoseira* species show that the CH_4 production depends on the species and is not proportional to the amount of organic matter (Table 2). Thus, *C. mediterranea* displays a BMP only slightly higher than that of *C. baccata* despite its higher organic matter (OM) content. This highlights that BMP may be strongly dependent on the composition of OM, e.g. phenolic compounds. The methane rate remains low compared with that of the red seaweed *G. manilaensis* (224 *N*m3 $CH_4.t^{-1}$) but close to *G. persica* (179 *N*m^3 $CH_4.t^{-1}$) [4].

Table 1. Metabolites contents in *C. baccata* and *C. mediterranea.*

Metabolite	***Cystoseira baccata***	***Cystoseira mediterranea***
Alginates	10.5g/100g dry weight	9,4/100g dry weight
Fucoidans	3.2g/100g dry weight	7,8g/100g dry weight
Lipids	1.97g/100g dry weight	1.84g/100g dry weight
Phenolic compounds	19.9 mg eq gallic acid/g dry weight extract	32. 2mg eq gallic acid/g dry extract
Flavonoids	11.1mg eq quercitin/g dry weight extract	15.6mg eq quercitin/ g dry extract
Tannins	29.1mg eq catechin/g dry weight extract	42.3mg eq catechin/g of dry extract
Total chlorophyl	0.28 mg/g of dry weight	0.25 mg/g dry weight
Carotenoids	0.10 mg/g of dry weight	0.11 mg/g dry weight
Fucoxanthin	0.65 mg/g of dry weight	0.71 mg/g dry weight

Table 2. Elemental composition and BMP yield of *C. baccata* and *C. mediterranea*

	Cystoseira baccata	***Cystoseira mediterranea***
Dry matter	73.0 % in raw material	89.0 % in raw material
Organic matter (OM)	49.0 % in raw material	67.0 % in raw material
C	32.6 % in raw material	32.4 % in raw material
N	2.2 % in raw material	2.5 % in raw material
H	4.5 % in raw material	4.4 % in raw material
S	1.4 % in raw material	1.1 % in raw material
BMP	168.0 *N*m^3 $CH_4.t^{-1}$ OM	174.0 *N*m^3 $CH_4.t^{-1}$ OM

Conclusion: Experimental results indicate that two *Cystoseira* specices from Moroccan coast are rich in secondary metabolites, such as fucoidans, alginates, polyphenols and fucoxanthin, which can be used for various applications, e.g., in cosmetics. Extraction residues can be used to produce methane through anaerobic digestion to promote sustainable and efficient production.

References

[1] 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.

[2]. Sellimi S. et al, Fucans from a Tunisian brown seaweed *Cystoseira barbata*: Structural characteristics and antioxidant activity, *Int. J. Biol. Macromol*., 66, (2014), 281-288.

[3]. Kord A. et al, Fatty acids composition of *Cystoseira sauvageauana* and *Laurencia pinnatifida* collected from the Algerian coast. *APTEFF*, 50, (2019), 1-352.

[4]. M.J. Hessami, et al. The bio-methane potential of whole plant and solid residues of two species of red seaweeds: *Gracilaria manilaensis* and *Gracilariopsis persica*. *Algal Research*, 42 (2019), 1015.

SD-OP10 ENHANCED CARBON CAPTURE AND BIOFIXATION USING FUNCTIONALIZED DEEP EUTECTIC SOLVENT AND *DESMODESMUS COMMUNIS* MICROALGAE

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Abstract: *This study explores the CO_2 capture with a customized deep eutectic solvent (DES) integrated with CO_2 biofixation by Desmodesmus communis. By efficient CO_2 desorption, nearly 90% was recovered. The DES-driven CO_2 capture enhances microalgal cultivation, boosting growth rates and biomass production. This research underscores the DES potential for sustainable microalgal biomass cultivation, contributing to CCUS strategies.*

Key words: CO_2 sequestration, CCUS, environmental sustainability, biomass

Introduction: Carbon capture technologies are crucial in addressing the escalating atmospheric CO_2 levels, consequence of anthropogenic activities. This study explores the integration of DES with microalgal-based CO_2 biofixation [1,2] as a promising approach for sustainable carbon capture and utilization.

Experimental: The DES consisted of chlorine chloride, ethylene glycol and monoethanolamine (ChCl:EG:MEA, 1:2:1 molar ratio) [3] and *D. communis* was cultivated in bioreactors under controlled conditions. CO_2 capture and desorption processes were conducted to evaluate the efficacy of the integrated system.

Results and discussions: CO_2 was efficiently captured in the tested DES, with subsequent desorption capacity. The approach demonstrated a significant increase in microalgal biomass production, with optical density (OD) showing a four time linear increase over 14 days in CO_2-treated cultures compared to controls. OD

Conclusions: This integrated approach showcases promising potential for efficient carbon capture and sustainable biomass production, offering a viable strategy for mitigating CO_2 emissions and fostering environmental sustainability.

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References:

[1]. Anyaoha, K.E.; Krujatz, F.; Hodgkinson, I.; Maletz, R.; Dornack, C. Microalgae contribution in enhancing the circular economy drive of biochemical conversion systems – A review. *Carbon Resources Conversion* (2024), *7*, 100203

[2]. Jin, X.; Gong, S.; Chen, Z.; Xia, J.; Xiang, W. Potential microalgal strains for converting flue gas CO2 into biomass. *Journal of Applied Phycology* (2021), *33*, 47-55

[3] .Brettfeld, E.G.; Popa, D.G.; Dobre, T.; Moga, C.I.; Constantinescu-Aruxandei, D.; Oancea, F. CO2 Capture Using Deep Eutectic Solvents Integrated with Microalgal Fixation. *Clean Technologies* (2024), *6*, 32-48

SD-OP11 EFFECT OF MICROWAVE-ASSISTED ORGANOSOLV PRETREATMENT ON FRUIT BY-PRODUCTS AS SUBSTRATES FOR FERMENTATION PROCESSES

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Key words: lignocellulosic biomass, food by-products, fermentation, biofuels

Introduction: Fruit pomaces resulted as by-products of food industry represent an important lignocellulosic biomass with high potential for valorization in biproducts to meet current societal needs. Due to their high sugar content, fruit pomaces, such as grape and apple pomaces show a huge potential to be transformed by fermentation processes in biofuels (bioethanol, biohydrogen and biomethane) as an alternative to fossil fuels, thus contributing to the transition to clean energy and a clean environment [1]. The production of biofuels from lignocellulosic biomass requires pretreatment, hydrolysis and fermentation steps, the pretreatment step being very important to break down the recalcitrant structure of lignocellulosic biomass and release the fermentable sugar [2].

Experimental: Here, the enzymatic extraction combined with microwave-assisted organosolv pretreatment was performed in order to extract the bioactive compounds from grape and apple pomaces and release the fermentable sugars to obtain biofuels. The enzymatic extraction was performed with pectinase in citric acid solution pH = 4.0, while the microwave-assisted extraction was performed in 50% hydroethanolic solution, at a solid liquid ratio of 1/15 (w/v), 1000 W microwave power, during 35 min., at 60 °C, with stirring. The liquid fraction was recovered by filtration and used for the recovery of the bioactive polyphenols, while the solid fraction was analyzed for cellulose, hemicellulose, lignin and extractible contents. The release of sugars from the lignocellulosic matrix was monitored by sugar composition (total sugars and reducing sugars by UV-Vis spectrophotometric assays and sugars profile by HPLC-CAD analysis).

Results and discussions: In Figure 1 the lignocellulosic composition and sugar content of both, raw (TSR) and pretreated grape pomaces (microwave pretreatment – TSR MAE and microwave and enzymatic pretreatments – TST MAE+P) is presented, highlighting the effect of the applied pretreatment on the recalcitrant structure of lignocellulosic biomass. After the pretreatment of grape and apple pomace it can be observed an increase in the content of cellulose and lignin and a decrease in the content of hemicellulose and extractible compared with the raw

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grape pomace. Also, the sugar composition of the pretreated biomass decreased, demonstrating the release of sugars in the liquid fraction.

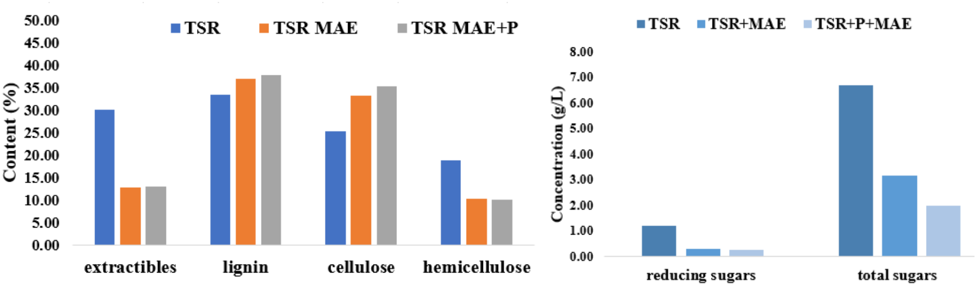

Figure 1. Composition of raw and pretreated grape pomace after the microwave and enzymatic extraction

Conclusions: The present work showed that the microwave-assisted organosolv pretreatment of grape and apple pomaces has a great potential to be used for the decomposition of the lignocellulosic structure with the aim of releasing sugars for fermentation processes to obtain biofuels. Further delignification process will lead to the complete disintegration of the lignocellulosic biomass to obtain high sugars yields and cellulosic biofuels.

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References:

[1] Leticia Eduarda Bender, Samuel Teixeira Lopes, et al., *Bioresource Technology Reports* 2022, 19, 101171, https://doi.org/10.1016/j.biteb.2022.101171

[2] Suncica Beluhan, Katarina Mihajlovski, Božidar Šantek and Mirela Ivancic Santek, *Energies* 2023, 16, 7003. https://doi.org/10.3390/en16197003

SD-OP12 ASSESSMENT OF HEAVY METALS CONTAMINATION OF SURFACE SEDIMENTS OF DANUBE RIVER

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***Abstract:**. The present research aims to assess heavy metal pollution in the lower Danube River basin, one of the largest European area of interest. Six heavy metals (Cd, Ni, Zn, Pb, Cu, Hg) were analyzed in two different seasons of 2023 (spring and autumn), using the X-Ray fluorescence spectrometry technique (EDXRF Spectro Xepos, Germany). The results of this research activity in the lower Danube River basin highlighted the presence of moderate metal (Ni and Zn) pollution and a low RI for the aquatic environment*

Keywords: Danube River, heavy metals, pollution indices.

Introduction: Heavy metals are present in the earth's environment. They are generated from anthropogenic and/or natural activities. Heavy metal pollution of soils and the environment is the result from industrialization, urbanization, and intensified irrigation water [1]. Six heavy metals (Cd, Ni, Zn, As, Cu, Hg) are the most frequently identified heavy metals in the environment, which, in high concentrations, are considered toxic to ecosystems and human health. [1].

Experimental part: Samples were selected to assess the level of heavy metals sediment contamination, to the existing pollution sources located the Danube River, between Mila 41 and Km 435.

The sediment samples were collected using a Van Veen Grab (area 0.04 m^2) and deposited in polyethylene recipients and kept at room temperature. Sediment samples were oven dried (24–48 h/105 °C), finely grounded, homogenized using a mortar grinder RM 200 (Retsch, Germany), and sieved with a 250-µm stainless steel sieve. Determination of heavy metals were analysed by X-Ray fluorescence spectrometry using an EDXRF Spectro Xepos spectrometer (Germany).

The results was validated using a Certicate of Certified Reference Materials-Stream Sediment NCS73022, Approved by China National Analysis Center for Iron and Steel (Beijing, China).

The assessment of heavy metal pollution is based on two correlated aspects: 1. a determination of the potential risks of heavy metals in sediments by calculating the Potential Ecological Risk Index (RI), and 2. an evaluation of the influence of anthropogenic activities on the level of heavy metal contamination in the surface sediments, using three specific pollution indices, the Geo–Accumulation Index (Igeo), the Contamination Factor (CF), and the Pollution Load Index (PLI)[2].

Results and discussions: The levels of heavy metals pollution in the Danube River was investigated based on following indices. The highest indices was Zn (moderate polluted), followed by Cd (low pollution).

The Ni and Cu pollution indices showed a low pollution levels, while As and Hg presented the lowest indices, that main a unpolluted sediment

Conclusions: The results of this research activity in the lower Danube River basin highlighted the presence of moderate metal (Ni and Cd) pollution and a low RI for the aquatic environment.

Acknowledgements:

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References:

[1] Kennedy O. Ouma, Agabu Shane, Stephen Syampungani., Aquatic Ecological Risk of Heavy Metal Pollution Associated with Degraded Mining Landscapes of the Southern Africa River Basins: A Review, Minerals, (2022), 12, 225.

[2] Dan Vasiliu, Andra Bucse, Naliana Lupascu, Bogdan Ispas, Catalin Gheablau, Ion Stanescu, Assessment of the metal pollution in surface sediments of coastal Tasaul Lake (Romania), Environ Monit Assess (2020) 192: 749.

SD-OP13 TOTAL MERCURY AND METHYLMERCURY CONCENTRATIONS IN MOLLUSKS COLLECTED FROM THE NW BLACK SEA SHELF (ROMANIA)

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Abstract: *This study provides information on the concentrations of mercury and methylmercury in mollusk samples collected from 15 stations (locatd at water depths of 13–149 m) from the NW Black Sea shelf. The mollusks were sampled in July 2023 on board the research vesel (RV) Mare Nigrum. The levels of total mercury concentration ranged from 25.7 to 184.9 µg/kg, whereas those of methylmercury concentration were in the range of 20.9–27.8 µg/kg.*

Keywords: Black Sea, mollusk, mercury, methylmercury.

Introduction: In recent years, contamination with toxic elements, *e.g.*, mercury (Hg) and methylmercury (MeHg) of marine organisms has been studied intensively due to the fact that these elements tend to bioaccumulate and pose human risks [1]. This pattern of trophic biomagnification arises from the increased bioavailability of the organic form of mercury (MeHg), which is readily absorbed and slowly eliminated. Hg is one of the most ubiquitous and persistent heavy metals that may occur naturally in the environment or derive from anthropogenic sources [2].

Experimental part: Samples of different mollusk species, including *Abra alba*, *Acanthcardia paucicostata*, *Anadara kagoshimensis*, *Cerastoderma glaucum*, *Ciona intestinalis*, *Lagis neapolitana*, *Modiolus adriaticus*, *Mytilus galloprovincialis*, *Pitar rudis*, *Polititapes aureus*, *Spisula subtruncata*, and *Upogebia pusilla* were collected from 15 sampling stations (located at water depths of 13–149 m) covering the NW Black Sea shelf. Mollusk samples were collected using a grab sampler with an opening mouth of 0.018 m on board the *RV Mare Nigrum*. The soft tissue was removed with a scalpel and placed in special glass vats for freeze-drying at -55 °C for 48 h using a freeze-dryer (ilShin BioBase, Netherlands). After lyophilization, samples were ground, sieved, and distributed according to each individual analysis. For MeHg extraction, 1.5 g of soft tissue was weighed, and each sample was transferred to a 50 mL polypropylene tube with screw caps and hydrolyzed with 10 mL of HBr (47%). After 5 min of stirring using a vertical mechanical shaker, 20 mL of toluene was added, the mixture was centrifuged (2400 rpm for 20 min), and then the supernatant, containing

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organomercury species, was collected in Falcon tubes. The whole procedure was repeated, and toluene (15 mL) was added again to the tube containing the tissue. The combined organic extracts were back-extracted twice with 6 mL of 1% (v/w) L-cysteine aqueous solution to strip MeHg from toluene. An aliquot of L-cysteine extract was then immediately analyzed [3]. Total Hg and MeHg concentrations were determined using a DMA 80 Milestone (Italy) automatic mercury analyzer by thermal decomposition of the solid sample and quantified by atomic absorption spectrophotometry according to EPA 7473 method.

Results and discussions: The levels of total Hg concentration (*THg*) in the mollusks collected from 15 stations were in the range of 25.7–184.9 µg/kg. Higher values of *THg* (>100 µg/kg) were measured in the species *Abra alba*, *Anadara kagoshimensis*, *Cerastoderma glaucum*, and *Modiolus adriaticus* at stations near Portita, Sfântu Gheorghe, and Constanta, whereas lower values (< 40 µg/kg) were found in the species *Lagis neapolitana*, *Pitar rudis*, *Polititapes aureus*, and *Upogebia pusilla*, at stations near Sulina, Sfântu Gheorghe, Constanta, and Mangalia. The levels of MeHg concentration (*MeHg*) in the species *Acanthcardia paucicostata*, *Modiolus adriaticus*, *Mytilus galloprovincialis*, *Pitar rudis*, and *Spisula subtruncata* collected from 2 stations near Constanta ranged from 20.9 to 27.8 µg/kg.

Conclusions: Higher levels of *THg* and *MeHg* were recorded in the Danube`s mouth area, due to the strong influence of the Danube’s input, and in Constanta area, due to the port activities.

Acknowledgements:

The research was financed by the Ministry of Research and Innovation - PN 23 30 01 03: "Improving the monitoring program of the Romanian Black Sea shelf in order to increase the capacity to evaluate and predict the impact of multi-stressors on marine ecosystem services" and 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".

References:

[1] González-Álvarez D., Jaramillo A. C., Muñoz N. C., Agudelo-Echavarría D. M., Soto-Ospina A., Ruiz Á. A., Total mercury and methylmercury levels in eggs from laying hens in a mining area in Bajo Cauca, Antioquia, Colombia, *Emerging Contaminants*, 9, 3, (2023), 100230.

[2] de Pontes G. C., de Carvalho Vicente M., Kasper D., Machado W. T., Wasserman J. C., Spatial distribution of total mercury and methylmercury in the sediment of a tropical coastal environment subjected to heavy urban inputs, *Chemosphere*, 312 (Part 1), (2023), 137067.

[3] Maggi C., Berducci M. T., Bianchi J., Giani M., Campanella L., Methylmercury determination in marine sediment and organisms by Direct Mercury Analyser, *Analytica Chimica Acta*, 641, 1-2, (2009), 32-36.

SD-OP14 PHYCOCYANIN LOADED ALGINATE-BASED HYDROGELS WITH POTENTIAL MEDICAL APPLICATIONS

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Abstract: *In this study novel phycocyanin alginate-based hydrogels were developed for possible wound healing applications. Firstly, phycocyanin, an antioxidant and antimicrobial compound, was obtained by microwave-assisted extraction from blue-green microalga. The release profile of the phycocyanin loaded in alginate-based hydrogels were evaluated in phosphate buffer solution at various pH values.*

Key words: phycocyanin, unconventional extraction methods, hydrogel, slow release

Introduction: *Spirulina platensis* is a blue-green microalga with important antioxidant properties [1, 2] and significant nutritional value (protein content comparable to the one of meat and soybeans, antioxidants [3], chlorophylls, and phycocyanin [4]). The antioxidant and antimicrobial activity of phycocyanin paired with a topical application of hydrogel patches loaded with the interest compound may lead to a new approach regarding wound healing.

Experimental: *Reagents:* Powdered spirulina (*Spirulina platensis* (lot 200616) retailed by Herbal Sana® and Blue Spirulina Powder marketed by Dragon Superfoods®), disodium phosphate, sodium dihydrogen phosphate monohydrate (Chemical Company SA Iasi), distilled water, polyvinyl alcohol (Mw 89000-124000, 87-89% hydrolyzed), sodium alginate, acrylamide, N,N′-methylenebis(acrylamide), and ammonium persulphate (Sigma Aldrich), were used for the microwave extraction process of phycocyanin and hydrogel synthesis.; *Determination of release rate:* The phycocyanin-based hydrogels were placed in phosphate buffer solution (PBS) of different pH values, at 37°C and the release of the interest compound was monitored over the course of nine hours to determine the influence of the pH on the release kinetic parameters.

Results and discussions: The highest phycocyanin concentration was obtained for the microwave-assisted extraction. The release rate of the interest compound

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exhibited little to no difference when the pH of the release medium (PBS) was varied from 6.50 to 8.90. The release kinetics shows a good fit to the Korsmeyer-Peppas model, with $R^2 = 0.987$ for pH = 6.5.

Conclusions: From the obtained data, phycocyanin was released from the hydrogel at a constant rate during the trials. The results obtained in our research show good potential for possible medical applications, considering the slow release of an antimicrobial compound.

Acknowledgements: This work was supported by a grant from the Romanian Ministry of Research and Innovation, CCCDI—UEFISCDI, project number PN-III-P2-2.1-PED- 2021-0273, within PNCDI III.

References:

[1] Romay C, Armesto J, Remirez D, González R, Ledon N, García I. Antioxidant and anti-inflammatory properties of C-phycocyanin from blue-green algae. Inflammation research : official journal of the European Histamine Research Society [et al]. 1998;47(1):36-41.

[2] Grover P, Bhatnagar A, Kumari N, Narayan Bhatt A, Kumar Nishad D, Purkayastha J. C-Phycocyanin-a novel protein from Spirulina platensis- In vivo toxicity, antioxidant and immunomodulatory studies. Saudi journal of biological sciences. 2021;28(3):1853-9.

[3] Lupatini AL, Colla LM, Canan C, Colla E. Potential application of microalga Spirulina platensis as a protein source. Journal of the science of food and agriculture. 2017;97(3):724-32.

[4] Miki W, Yamaguchi S, Konosu S. Carotenoid composition of *Spirulina maxima*. Bulletin of the Japanese society for the Science of Fish. 1986;7:1225.

BOOK OF ABSTRACTS

SICHEM – 2024

D – Green applied chemistry and agro-resources valorization (GACARV)

3. Poster presentations

SD-P01 STUDIES ON BIOSURFACTANT PRODUCTION BY *BACILLUS MYCOIDES* STRAIN

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Abstract: *Currently, there is a growing interest in exploring microorganisms and substrates for the production of significant amounts of biosurfactants due to the growing demand for these biocompounds in industrial and environmental applications. This study was carried out to evaluate the ability of the Bacillus mycoides strain to produce biosurfactants and to determine a suitable substrate for their production. Two carbon sources, including waste cooking oil (2%) and whey (2%), were used as different low-cost substrates in the biosynthesis processes. Biosurfactant production was monitored by measuring the emulsification index (E_{24}). Whey proved to be the best substrate for biosurfactant production, followed by waste cooking oil. The TLC chromatographic analysis revealed that the microbial surfactants produced by the Bacillus mycoides strain were lipopeptides. Therefore, this strain represents an important biosurfactant producer, and the application of its bioproducts in bioremediation or industrial sectors should be exploited.*

Key words: biosurfactant, *Bacillus mycoides*, cheap substrates, lipopeptides

Introduction: Research on the synthesis of bacterial biosurfactants has increased in recent years, due to their important properties, such as high temperature and salinity tolerance, stability in pH variation, high degradation rate, better selectivity and less toxicity [1,2].

Experimental and/or Modelling: Biological material - *Bacillus mycoides* strain. Culture media: the strain was grown on nutritive agar medium (pre-inoculum), with the following composition % (g/v): meat extract 3.0, bacto-peptone 1.0, NaCl 5.0, and agar 2.0; biosynthesis media: M1 liquid medium (%) (g/v): waste cooking oil 2.00, as carbon source, and corn extract 2.00, as nitrogen source; M2 liquid medium (%) (g/v): whey 2.00, as carbon source, and corn extract 2.00, as nitrogen source. Bioprocess conditions: 30ºC, initial pH 7.0-7.5, 72 hours, 220 rpm, and inoculation volume 10%. The emulsification index (E_{24}) was calculated by the ratio between the height (mm) of the generated emulsion and the total height (mm) of the mixture, multiplied by 100. The experiments were performed in triplicate.

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Results and discussions: The supernatants obtained at the end of the bioprocesses were evaluated for their capacity to emulsify the sunflower oil, heptane, and octane. The values of the emulsification index (E_{24}) obtained in the case of M1 medium were 67.37% for heptane, 68.96% for octane, and 66.53% for sunflower oil. The results obtained with M2 medium containing whey as a carbon source were higher compared with M1 medium, with an emulsification index of 72.22% for heptane, 69.23% for octane, and 64.81% for sunflower oil. The emulsions were stable for more than one month in both cases. The partially purified bioactive compounds were analyzed by the TLC method, which indicated the nature of the biosurfactants produced as lipopeptides.

Conclusions: The results obtained demonstrate that *Bacillus mycoides* strain could be attractive for use in biosurfactants production, these bioproducts being useful for bioremediation and industrial biotechnology applications.

References:

[1] Schalchli H., Lamilla C., Rubilar O., Briceño G., Gallardo F., Durán N., Huenchupan A., Diez M.C., Production and characterization of a biosurfactant produced by *Bacillus amyloliquefaciens* C11 for enhancing the solubility of pesticides, *J. Environ. Chem. Eng.*,11 (6), (2023), 1-11, https://doi.org/10.1016/j.jece.2023.111572.

[2] Ali F., Das S., Hossain T.J., Chowdhury S.I., Zedny S.A., Das T., Ahmed Chowdhury M.N., Uddin M.S., Production, optimization, stability and oil emulsifying potential of biosurfactants from selected bacteria isolated from oil-contaminated sites, *R. Soc. Open Sci.* 8, 211003, (2021). https://doi.org/10.1098/rsos.211003

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SD-P02 NEW ELECTRODES PREPARED THROUGH THE RECYCLING OF ANODIC PLATE OF THE SPENT LEAD - ACID BATTERIES

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Abstract: *Lead acid batteries are used in worldwide at automobiles due to their low cost and high energy density. The number of spent lead acid batteries has increased because the comfort of driving has become a daily habit. The management of the green chemistry includes the necessity of recycling of spent electrodes in the context of new electrodes in the environment of origin. In this paper the context of a new life cycle of anodic electrode from spent car battery is detailed and demonstrated. The recycling method is friendly with the environment. The structure of the prepared samples was analyzed by X - ray diffraction (XRD) data, Fourier – Transform Infrared spectroscopy (FTIR) and UltraViolet – Visible spectroscopy (UV-Vis) spectra. The electrochemical perfrmances of the new electrode materials were demonstrated by cyclic voltammograms.*

Key words: recycling, anodic plate, XRD, FTIR, CV, electrode, batteries

Introduction: The lead acid batteries are widely used in the automotive industry due to their low production cost. Recycling of secondary sources is an important component of the life cycle and circular economy of products and materials. Secondary lead from spent car batteries is an important point in the recycling industry. The most important aspect in the development of new electrodes for automotive batteries is to reformulate and to simplify the chemical composition of the electrodes in order to facilitate the recycling processes after their use [1].

Experimental Procedure: Vitreous system in the $x\mathrm{CaO}\cdot5\mathrm{Fe_2O_3}\cdot(95-x)\mathrm{Pb}$ composition where $x = 0 – 50$ mol% CaO were prepared by melt – quenching method using as raw materials: the anodic plate of spent car battery as source of lead, calcium oxide and iron trioxide powders. Samples were characterized by XRD, FTIR and UV-Vis data and cyclic voltammograms.

Results and discussions: Analysis of the XRD data indicates vitroceramics with varied crystalline phases for samples with $x \leq 20$ mol% CaO and amorphous structures at higher CaO levels. FTIR data indicate that the increasing of the CaO content in the host matrix leads to the decrease of intensities of the IR bands corresponding to the sulfate units. The UV-Vis bands provide relevant information about the electronic transitions of the Pb^{+2}, Fe^{+2} and Fe^{+3} ions. Cyclic voltammograms have well - defined peaks for samples with x = 10, 20 and 30 % CaO.

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Conclusions: Electrode materials were prepared la 1050 ^oC from spent anodic plate of a car battery. The adding of higher CaO content in the host matrix produces the desulphurization of the new material.

References:

[1] Xiaofeng Gao, Yiran Zhou, Mengqi Fan, Min Jiang, Manli Zhang, Hongying Cai, Xiaoming Wang. "Environmental risk assessment near a typical spent lead-acid battery recycling factory in China." *Environmental Research* 233 (2023): 116417.

SD-P03 REUTILIZATION OF CONSTRUCTION AND DEMOLITION WASTE AS COMPOSITES IN CEMENT MATERIALS

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Abstract: *At production of the cement raw materials can be partially substituted by regenerable waste provided from glasses, construction and demolition waste in order to reduce environmental problem and burden of landfills. In this study the composites were synthetized using as raw materials construction and demolition waste by incorporation in the glasses. Structure and mechanical properties of the composite - cement materials have been studied by the analysis of X - ray diffraction (XRD), Fourier – Transform Infrared (FTIR) and Nuclear Magnetic Resonance (NMR) spectra and Vickers hardness data. The results indicate new possibilities to use 2.5 % amounts of composites in cement paste because promote the formation of C-S-H network which provides strength and long stability of the cement paste.*

Key words: construction and demolition recycling, composites, cement, XRD, FTIR, NMR, Vickers hardness

Introduction: In the world, the Portland cement manufacture occupies the third – largest industry in terms of energy consumers and emits 7 % of the total CO_2 emissions in the atmosphere. The development of other class of cement - based materials as a viable alternative to a circular economy must occupy research in the field in according to the European Union. The use of renewable raw materials such as coal gangue, construction and demolition waste, fly ash, metallurgical waste, glasses is a solution for a circular economy [1]. This paper is focused on the valorization of construction and demolition waste as raw material in new cement products.

Experimental Procedure: New composites were synthetized using as raw materials glass waste and lime, brick, ACC, mortar or plaster waste by wet synthesis method. The composite – cement materials were prepared using the *water:cement* ratio of 0.3:1 and 2.5 % weight of composite in the cement amount. Samples were characterized by XRD, FTIR, NMR and Vickers hardness data.

Results and discussions: Analysis of the XRD data indicates the presence of calcium silicates phases, $CaCO_3$ and $Ca(OH)_2$ crystalline phase. The IR spectra reveal that the addition of composites in the cement material did not delay the formation of C-S-H gel and $Ca(OH)_2$. Numbers of carbonates units and water in composite – cement materials were also increased. NMR signal can be categorized by their size and can be resolved into four discrete populations of water. The values

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of Vickers hardness of the composite - cementing materials were higher as compared to control cement.

Conclusions: This study seeks to synthesize an improved cement - based material with 2.5% limestone – silicate composite in view of applications as substitute for cement in the constructions.

References:

[1] Z. Liu, C. Shi, Q. Shi, X. Tan, W. Meng, ”Recycling waste glass aggregate in concrete”. *J. Cleaner Production* 370 (2022): 133545

SD-P04 THE DEVELOPMENT OF NEW BLACK SOLAR ABSORBERS BASED ON IRON – STABILIZED ZIRCONIA CERAMICS

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Abstract: *Solar absorbers are a key component to the performance of various solar thermal systems such as solar thermal power plants and solar thermo-photovoltaics. The aim of this work was to explore the structure of the vitroceramic system with the* $xFe_2O_3{\cdot}(100\text{-}x)[ZrO_2{\cdot}MgO]$ *composition where* $x = 0$ *- 40mol%* Fe_2O_3*. Obtained samples were characterized by investigations of analysis of X - ray diffraction (XRD), Fourier – Transform Infrared (FTIR), UltraViolet – Visible (UV-Vis), Photoluminescence (PL) and Electron Paramagnetic Resonance (EPR) spectra. Increment of* Fe_2O_3 *content has a substantial effect on the promoting of the thermal and solar to thermal efficiencies of the zirconia composites.*

Key words: ceramics, black zirconia, absorbers, XRD, FTIR, UV-Vis, PL and EPR spectroscopy.

Introduction: Solar energy is one of the most promising renewable energy options among those available for achieving a considerable amount of energy - saving and carbon emission reduction and for the replacing fossil fuels because can created electrical energy and heat without polluting the earth. For the first time in the 2015 year the optical properties of black zirconia are investigated for the solar applications [1]. Black zirconia ceramics have many problems, such as uneven color and poor phase stability. In this paper zirconia ceramics doped with the varied Fe_2O_3 contents were prepared by a high temperature solid state reaction process.

Experimental procedure: The samples having $xFe_2O_3{\cdot}(100\text{-}x)[ZrO_2{\cdot}MgO]$ composition where $0 \leq x \leq 40$ mol% Fe_2O_3 were prepared at 1300 °C. MgO has role of stable agent of the tetragonal and / or cubic ZrO_2 phase while Fe_2O_3 act as both stable agent and activating agent due to its lower melt temperature**.** Samples were characterized by XRD, IR, UV-Vis, PL and EPR data.

Results and discussion: X-ray diffraction patterns confirm the presence of four crystalline phases, namely tetragonal and monoclinic ZrO_2, MgO and Fe_3O_4 crystalline phases with cubic structures, respectively. The IR data demonstrate that the addition of Fe_2O_3 improves the tetragonal / cubic ZrO_2 content by decreasing of monoclic ZrO_2 phase but appear new IR bands corresponding to the stretching vibrations of the Fe-O bonds from $[FeO_4]$ and $[FeO_6]$ structural units. UV-Vis and PL data indicate larger concentrations of oxygen vacancies with addition of higher Fe_2O_3 concentrations. The EPR spectra are due to the presence of Fe^{3+} ions and depend on the Fe_2O_3 content of samples.

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Conclusions:

Our investigations shows that the best result was obtained for the sample containing 40 mol% Fe_2O_3 which a recommends as suitable as solar absorbers.

References:

[1]. H. Lv, J. Bao, F. Ruan, F. Zhou, Q. Wang, W. Zhang, W. Guo, Y. Zhang, X. Song, S. An, Preparation and properties of black Ti - doped zirconia ceramics. ***J. Mater. Res. Technol***. 9(3) (**2020**): 6201-6208.

SD-P05 RECOVERY OF ELECTRODES FROM USED CAR BATTERIES BY RECYCLING AND DOPING THEM WITH METAL OXIDES

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Abstract: *Currently, lead recycling methods in car batteries are sophisticated, costly and polluting. The purpose of the work is the recycling through a simple and eco-innovative technology of the active mass from the plates of the used battery electrodes, the incorporation of metal oxides in view of applications as new products in the car battery. The topic proposed for this paper includes comparative analysis of the structure and electrochemical properties of vitreous system in the* $xCuO·5MnO_2·(95x)Pb$ *composition where x = 0 – 40 mol% CuO from X - ray diffraction (XRD), InfraRed (IR), Electron Paramagnetic Resonance (EPR) data and cyclic voltammograms. Our results indicate that by doping with 5 mol% CuO the structure of the vitroceramics and electrochemical performances were improved.*

Key words: car battery recycling, XRD, IR, EPR, CV, electrode materials.

Introduction: A lead - acid battery is a rechargeable battery that uses Pb at anodic plate, PbO_2 at cathodic plate and sulfuric acid as electrolyte solution. Lead is immersed in sulfuric acid to allow a controlled chemical reaction. This chemical reaction is what causes the battery to produce electricity. Then this reaction is reversed to recharge the battery. The oxygen in the water reacts with lead sulfate on the positive plates to convert them back into PbO_2, and oxygen bubbles rise from the positive plates when the reaction is almost complete [1].

Experimental procedure: The samples having $xCuO·5MnO_2·(95x)Pb$ composition where x = 0 – 40 mol% CuO were prepared by melt quenching method at 950 °C using as starting materials: anodic electrode from a spent car battery, CuO and MnO_2 powders. Prepared materials were investigated by XRD, IR, EPR and VC data.

Results and discussion: XRD data show vitroceramics for all samples containing different crystalline phases. The addition of 5 mol% CuO in the host matrix yields a process of partial desulphurization of the spent anodic plate. For higher CuO levels there was an interconversion of varied oxo - sulphatized phases of the lead. The analysis of IR data shows that the intensities of the bands assignment of sulphate and sulphite units were decreased for sample with 5 mol % CuO comparatively with undoped and doped samples with a higher content of metal oxides. The EPR data evidence the resonance signals corresponding to the Mn^{+2} and Cu^{+2} ions. Cyclic voltammograms reveal that the current density increases for the sample with 5 mol% CuO.

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Conclusions: Combining the results for varied methods we can conclude that the best result was obtained for the sample containing 5 mol% CuO which a recommends as suitable as new electrode for lead accumulator.

References:

[1]. A.V. R. Kumar, Ch. S. Rao, N. N. Rao, V. R. Kumar, I. V. Kityk, N. Veeraiah, J. Non-Cryst. Solids 358 (2012) 1278.

SD-P06 OBTAINING MICROBIAL INULINASE BY *ASPERGILLUS* SP. FOR THE PREVENTION OF METABOLIC AND NUTRITIONAL DISEASES

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Abstract: *In the current scientific context, digestive health researchers have proposed that microbial inulinase supplementation may improve dietary fructan digestion in the stomach. Fructans comprise fructose residues, typically with a sucrose (glucose-fructose) residue at the terminal end. By breaking down fructan into fructose, it can be more easily absorbed by the upper intestine. This stops fermentation in the lower intestine, which would lead to uncomfortable digestive symptoms like bloating, cramps, and gas, especially in people who are intolerant of fructan or have irritable bowel syndrome. Inulinases are an important class of enzymes used in many fields, especially in the food and pharmaceutical industries, to produce fructose. Microbial inulinases are important in the hydrolysis of inulin and the production of fructose and fructo-oligosaccharides (FOS). Different microbial strains are responsible for producing these enzymes. For inulinase production, the most commonly used species are Aspergillus sp. and Kluyveromyces sp. For efficient use in the intended purpose, a microbial biotechnological strategy was developed to obtain reproducible yields of the microbial inulinase with a strain belonging to the genus Aspergillus located in the Collection of Microorganisms of Industrial Importance of the National Institute of Chemical and Pharmaceutical Research and Development, ICCF (CMII), grown on a fermentation medium based on different carbon sources (inulin and agro-food by-products). The crude extract was purified by fractional precipitation with ammonium sulfate, and the resulting precipitate was dissolved and dialyzed. After biosynthesis, the fermentation medium yielded a solution with an inulinase content of 92.2 U/ml, a specific activity of 164.6 U/mg protein, and a yield of 30%. To gain additional benefits for delivery and application, such as enzyme protection from protease degradation, pH changes, improved bioavailability, and controlled release, inulinase must be encapsulated in liposomes or immobilized on various polymeric supports, increasing its stability.*

Key words: Inulinase, *Aspergillius species*, biosynthesis, inulin, fructose, nutritional diseases.

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SD-P07 STUDY OF HEAVY MINERALS CONCENTRATIONS IN SEDIMENTS FROM SEVERAL SECTORS OF THE LOWER DANUBE RIVER

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***Abstract**: For provenance and mineralogical complex description we analysed 45 sediment samples that were collected from 15 profiles of the Lower Danube River. Heavy mineral fractions were extracted using specific techniques and analyzed to determine the origin of the sediments.*

Key words: heavy minerals, sediments provenance, mineral associations, Danube River

Introduction: The Romanian part of the Danube River is an important watercourse which plays a pivotal role in shaping the geomorphology and sediment dynamics of the surrounding regions [1]. This study sought to examine the composition, distribution, and origin of heavy minerals in the sediments of the Lower Danube River in April 2023. It also aimed to uncover the geological mechanisms that have impacted the deposition and dynamics of sediment.

Experimental part: In total, 45 samples were collected using a Van Veen grabber from predetermined locations where sandy sediments are expected to be found for further mineralogical analysis. From each sample it was extracted 100g of dried sediment to be analyzed in the mineralogical laboratory. After drying and sieving, the proportion of coarse (>1mm), medium (0.063-1mm), and fine (<0.063mm) fractions were noted. The 0.063-1mm fraction was further processed for mineralogical analysis, comprising the following procedures: treatment with approximately 15% HCl for removal of the carbonates, followed by rinsing, drying, and weighing to determine the carbonate fraction removed. The organic fraction was eliminated using 35% H_2O_2, then again rinsing, drying, and weighing for organic matter determination. Subsequent gravitational separation using SPT (sodium polytungstate, 2.8 g/cm^3) solution, yielding in differentiation of heavy and light mineral fractions. The heavy fraction was analyzed for mineral composition and roundness characteristics using a binocular microscope [2].

Results and discussions: Findings suggest the prevalence of several key heavy minerals, such as zircon, tourmaline, garnet, epidote, disthene, rutile, and amphiboles, among others. These minerals exhibit distinct morphologies and compositions, reflecting their diverse origins from both local and distant geological formations. By comparing the mineral assemblages found in the sampled sediments it was intended to understand the contributions of various tributaries and one or several geological formations that represents the potential source rocks, and also a specific provenance area.

According to the component concentrations of the heavy minerals found within our analyzed samples:

i. it has been determined that the garnet-hornblende-disthene-epidote association is dominant (50.71%);

ii. most likely, the source rocks are represented by the metamorphic rocks of the Southern Carpathians, which contribute significantly through the left tributaries of the Danube.

Conclusions: The study emphasizes the need for continuous research to refine our understanding of sediment sources and transport patterns.

It also underscores the importance of interdisciplinary approaches in addressing complex environmental challenges and guiding sustainable river management practices in the Romanian Danube basin.

The Danubian sediments analysed in the surveyed sectors are having a South Carpathian origin, as their provenance are represented by the lower-to-medium grade metamorphic rocks. The main assemblage included by the sedimentological material comprise minerals formed in high temperature and medium pressure conditions.

References:

[1] Panin N., 1977. Sedimentologia. In: Istoria ştiintelor Geologice în România, Editori: S.Ştefãnescu, G.Murgeanu, V.Mihãilescu, p.46-53, Ed.Acad.Rom., Bucureşti

[2] Pojar I., Gheablău C., Șeclăman M., Melinte – Dobrinescu M., 2019: Heavy mineral abundances in the Lower Danube Tributaries. Geo-Eco-Marina, No. 25.

Acknowledgements

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SD-P08 *CLADOPHORA VAGABUNDA* ALGAE AS A SUSTAINABLE SOURCE OF NEW CELLULOSE NANOFIBERS

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Short Abstract: *In this study, the extraction of cellulose nanofibers from Cladophora vagabunda was performed by precipitation with ethanol.*

Key words: *Cladophora vagabunda*, polysaccharides, ethanol.

Introduction: Biodegradable polymers such as polysaccharides (cellulose, starch) can be obtained through different chemical syntheses from *Cladophora vagabunda* algae found along the Romanian Black Sea Coast. Biodegradable biopolymers represent a large current field of research with important implications in the chemical, food, cosmetic, pharmaceutical and agronomy industries.

Experimental: Fresh *Cladophora vagabunda* algae was harvested from the north of the Romanian Black Sea Coast. The seaweeds were washed with sea water, distilled water and cleaned of impurities. Then were placed for 2 days in a dehydrator with 5 overlapping trays, where they dehydrate evenly. Subsequently, the dried algae were finely ground by mortaring. To extract cellulose from *Cladophora vagabunda species*, 10 g of algae were introduced into a solution of ethanol. The extraction was performed in a Soxhlet extractor. Then, the following substances were added in different concentrations: sodium hydroxide, ammonium oxalate, acetic acid and hydrochloric acid for bleaching.

Results and discussions: The dried algae and the dry cellulose extracted from algae were subjected to observation by transmission under the SEM TM4000 Tabletop SEM microscope (Hitachi, Japan). In order to highlight the functional groups of species in the *Cladophora vagabunda* algae sample, the equipment for FTIR - Tensor 37 Bruker analyses (Woodstock, NY, USA) was used.

Conclusions: A yield of 17.42 % wt cellulose per DM was obtained proving that *Cladophora vagabunda* species is a viable alternative resource in cellulose production.

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SD-P09 OPTIMIZING THE CONDITIONS OF THE FERMENTATION PROCESS OF ROCKWEED-BASED COMPOST

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Abstract: *Compost tea (CT) was prepared from compost derived from rockweed (Ascophyllum nodosum) residue, which fermented in water. The effects of fermentation process factors, i.e., water/compost mass ratio (4.2–9.8 g/g) and fermentation time (4.2–9.8 d = 100–236 h) on the contents of nitrogen (1.090 ± 0.050%), phosphorus (21.72 ± 6.44 mg/kg), and potassium (0.439 ± 0.138%) of CT were quantified using quadratic polynomial equations. Optimal levels of process factors (4.2 g/g and 7 d = 168 h) were identified based on desirability function approach. CT produced at optimal levels of process factors will be tested for lettuce germination.*

Key words: compost fermentation, compost tea, modeling, optimization, rockweed (*Ascophyllum nodosum*).

Introduction: CT is a filtrate obtained from compost fermented in water. It is either aerated (prepared from a compost-water slurry that was aerated during the fermentation process) or non-aerated (prepared from a compost-water slurry that was not aerated or received minimal aeration only at the initial mixing stage of the fermentation process) [1–3]. Due to its composition, especially macronutrients, micronutrients, humic acids, phytohormons, and beneficial microorganisms, CT can significantly improve the growth, yield, and quality of edible and ornamental plants as well as reduce the incidence and severity of plant pests and diseases [1–4]. These effects depend on different factors, including type of compost, fermentation conditions, application method of CT, and type of plant.

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Experimental and modelling: Non-aerated CT was prepared from compost obtained by composting rockweed residues with LECA (lightweight expanded clay aggregate) in a tumbler. The compost-water suspension was stirred once at the beginning of fermentation and then left in the dark at 25 °C. At the end of the experiment, the broth was filtered through cheesecloth and the filtrate (CT) was analyzed. According to a Central Composite Design (CCD), 12 experiments were performed at five levels of each process factor (independent variable), *i.e.*, water/compost mass ratio (R_m = 4.2–9.8 g/g) and fermentation time (t = 4.2–9.8 d). The contents of nitrogen ($N = 1.090 \pm 0.050\%$), phosphorus (P = 21.72 ± 6.44 mg/kg), and potassium ($K = 0.439 \pm 0.138\%$) were selected as process responses (dependent variables). The effects of process factors on its responses were quantified using quadratic polynomial equations.

Results and discussions: Process responses were predicted using the statistical models described by Eqs. (1)–(3), where the regression coefficients were determined from experimental data. The optimization of fermentation process factors, aiming at maximizing the process responses, was based on desirability function approach. Optimal levels of process factors were $R_{m,opt}$ = 4.2 g/g and t_{opt} = 7 d. To validate the statistical models, 3 fermentation tests were performed at optimal levels of process factors. The mean levels of experimental responses for these 3 tests (N_{opt} = 1.12%, P_{opt} = 34.3 mg/kg, and K_{opt} = 0.76%) and the values of predicted responses at $R_{m,opt}$ and t_{opt} ($N_{pr,opt}$ = 1.13%, $P_{pr,opt}$ = 33.7 mg/kg, and $K_{pr,opt}$ = 0.83%) were not significantly different ($p > 0.23$ for unequal variance t-test), which proves the validity of statistical models. CT produced at optimal levels of process factors will be tested for lettuce germination.

$$N_{pr} = 1.000 - 0.039R_m + 0.003R_m^2 + 0.069t - 0.004t^2 - 0.002R_mt \quad (1)$$

$$P_{pr} = 37.22 - 7.958R_m + 0.319R_m^2 + 7.176t - 0.567t^2 + 0.057R_mt \quad (2)$$

$$K_{pr} = 1.082 - 0.238R_m + 0.013R_m^2 + 0.120t - 0.007t^2 - 0.002R_mt \quad (3)$$

Conclusion: Recycling rockweed residues using composting and compost fermentation could have significant beneficial agronomic and environmental effects.

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References:

[1] Pilla N., Tranchida-Lombardo V., Gabrielli P., Aguzzi A., Caputo M., Lucarini M., et al., Effect of compost tea in horticulture, *Horticulturae*, 9, 9, (2023), 984.

[2] Scheuerell S., Mahaffee W., Compost tea: Principles and prospects for plant disease control, *Compost Science & Utilization*, 10, 4, (2002), 313–338.

[3] St. Martin C. C. G., Brathwaite R. A. I., Compost and compost tea: Principles and prospects as substrates and soil-borne disease management strategies in soil-less vegetable production, *Biological Agriculture & Horticulture*, 28, 1, (2012), 1–33.

[4] Jarboui R., Dhouib B. Ammar, E., Effect of food waste compost (FWC) and its non-aerated fermented extract (NFCE) on seeds germination and plant growth, *Open Journal of Soil Science*, 11, 02, (2021), 122–138.

SD-P10 HYBRID GREEN EXTRACTION OF PHYTOEXTRACTS FROM *HEDERA HELIX* L

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Abstract: *The aim of this research was to investigate how the hybrid methods affects the extraction effectiveness of bioactive compounds from Hedera helix L. Hybtrid extraction with combined microwaves and ultrasounds (UMAE) was selected due to its potential to enhance extraction efficiency while reducing solvent and energy consumption. The best results were achieved for the phytoextracts obtained by UMAE.*

Key words: Ultrasound, Microwave, *Hedera helix L,* polyphenols, antioxidat activity

Introduction. Ivy (*Hedera helix* L.) is a medicinal plant, which belongs to the Araliaceae Juss. Family. This plant exhibits respiratory, anti-inflammatory, immunostimulatory, antimicrobial, antithrombin, and antimutagenic activities.

Methods. The innovative equipment used for the UMAE of phytocompounds from *Hedera Helix* was described by Calinescu et al [1]. The extraction of phytocompounds from *Hedera Helix* was performed by different methods: conventional extraction and UMAE, using water as solvent. Various parameters such as ultrasound power and microwave power, plant-to-solvent ratio, and ethanol concentration in the extraction solvent were examined to identify the factors affecting the extraction process.

Conclusions. The extraction efficiency was evaluated by analysis of the total content of saponins, carbohydrates, polyphenols, but also the antioxidant capacity of ivy leaves extracts. For saponins extractions the highest value of TSC was obtained by UMAE (TSC_{UMAE} = 99.19±1.13 mg DE/gDM). As for carbohydrates and polyphenols, the best results were achieved by UMAE (TCC = 254.17±8.53 mg GE/gDM and TPC= 33.02±0.75 mg GAE/gDM).

Acknowledgement

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References

[1] Calinescu, I.; Vinatoru, M.; Ghimpeteanu, D.; Lavric, V.; Mason, T.J. A new reactor for process intensification involving the simultaneous application of adjustable ultrasound and microwave radiation. Ultrason. Sonochem. 2021, 77, 105701.

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SD-P11 UTILIZATION OF PLANT WASTE AND BIOMASS FROM THE MEDICINAL PLANT USING MODERN MICROWAVE TREATMENT TECHNIQUE

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Abstract: *Plant biomass and plant waste can generate minerals, chemical compounds, materials and fibers for industry, solid fuels for small households, feed for animal husbandry. Biomass and plant waste can be provided by agricultural by-products, municipal, forestry, wood processing and plant and plant product processing industry. This research concerns plant biomass and plant waste from the industrial production of medicinal plants and food supplements. For the waste from the production sections, an analysis of their composition and a characterization of each individual waste will be made in order to establish the best method of valorization. For the chemical analysis of the composition of these wastes, a preliminary treatment with microwaves was used, which, thanks to the radiant energy it propagates, creates, from the inside, a pressure on the cell wall of the plant, which stretches and, finally, breaks. From the multitude of medicinal plants generating vegetable waste, we selected 2 plants: mint, Mentha piperita and passionflower, Passiflora incarnata, which we analyzed as waste. The two plants chosen for waste analysis were selected because, in industrial extraction, the solvent used is water, a cheap and accessible solvent, which makes industrial extraction sustainable, at large volumes of work. At the same time, the high cost of the thermal energy used in industrial extraction leads us to the working hypothesis, that, following the research activity, we will find additional possibilities of superior valorization of the resulting vegetable waste. A first measure for the valorization of plant waste is their treatment with microwaves in solvent water or 0.5 N NaOH solution, for the delignification of the waste and the determination of the soluble lignin content and to successfully carry out the enzymatic hydrolysis of the waste, obtaining sugars, which offers a perspective of superior recovery of this waste. Lignin is one of the most widespread natural polymers of plant biomass and plays a crucial role in the structure of woody plants. This gives strength and rigidity to plants, allowing them to support their weight and withstand adverse environmental factors. For this reason, in the field of biomass, determining the content of soluble/insoluble lignin is an essential step in understanding the composition and quality of plant biomass. For the mint and passion flower wastes, chosen for the analysis, after the microwave treatment for their delignification and the dosage of the soluble lignin content, physico-chemical analyzes were carried out to determine the evaporation residue, the extractable substances and the determination of the active principle content, namely:- dosage of the content of flavones, expressed in vitexin, for the passiflora waste,- dosage of the content of total polyphenols, expressed in chlorogenic acid, for the mint waste.*

The major objective of the research activity carried out in the present study was to find the solutions to use all plant waste and plant biomass from the ***Hofigal*** *organization, so as to obtain a superior valorization of this waste, in order to provide horizontal industrial production with new cheap sources of raw materials, replacing expensive imports, stopping the deforestation of wood mass and thus contributing to the protection of the environment, to the reduction of the energy crisis, the crisis of raw materials and food, which have manifested themselves in recent years and which are manifested even now, worldwide.*

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SD-P12 PEELABLE HYDROGELS INCORPORATING SILVER-DECORATED CARBON NANOFIBERS FOR IMMEDIATE BIOLOGICAL DECONTAMINATION

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Abstract: *This study presents the synthesis and characterization of peelable nanocomposite hydrogel films, reinforced by carbon nanofiber-supported silver nanoparticles with remarkable antimicrobial properties against Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa. These materials are suitable for immediate decontamination applications, designed as fluid formulations that can be applied on contaminated surfaces. Subsequently, they can rapidly form a peelable film via divalent ion crosslinking and can be easily peeled and disposed of.*

Keywords: decontamination, nanocomposite, hydrogel, antimicrobial activity, ionic crosslinking

Introduction: The recent pandemic instigated by SARS-CoV-2, alongside the looming threat of chemical warfare, underscores the critical necessity for enhanced protective measures and decontamination techniques, vital for addressing the proliferation of biological contaminants, which pose a significant risk to global health security [1-3]. The study indicates that using oxidized carbon nanofibers as a substrate for the production of silver nanoparticles results in a significant improvement of their antimicrobial efficacy. Specifically, the silver nanoparticles generated in the presence of the nanofibers exhibited much stronger antimicrobial properties compared to those produced without the nanofibers. These findings suggest that utilizing oxidized carbon nanofibers as a substrate for silver nanoparticles could be a promising approach for enhancing their antimicrobial activity. Subsequently, sodium alginate was incorporated into the decontaminating formulations to enable the formation of ionic crosslinks in the presence of divalent ions. This addition of sodium alginate played a crucial role in enhancing the efficiency of the decontamination process by enabling the formation of a cohesive

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crosslinked network, which effectively entraps the contaminants into the polymeric matrix and can be easily peed off the decontaminated surface.

Experimental: *Reagents:* Polyvinyl alcohol (PVA, average Mw 85.000–124.000 Da, 87–89% hydrolyzed), carbon nanofibers (CNF, D × L 100 nm × 20–200 μm), nitric acid (HNO_3, 68%), sulfuric acid (H_2SO_4, 95–98%), sodium hydroxide (NaOH), silver nitrate ($AgNO_3$), sodium borohydride ($NaBH_4$). *Methods:* The synthesized materials were characterized via TEM, rheological measurements, and tensile tests. Microbiological analyses assessed the decontamination efficacy against *Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa*.

Results and discussions: The inclusion of oxidized carbon nanofibers during the process of nanoparticle synthesis results in a reduction of silver particle size. This phenomenon can be ascribed to the oxidized carbon nanofibers acting as an anchoring site for the nucleation and subsequent growth of the silver nanoparticles. The presence of polar functional groups on the surface of the carbon nanofibers facilitates this process. The morphology and size of the nanoparticles were assessed by transmission electron microscopy (TEM) – Fig.1.

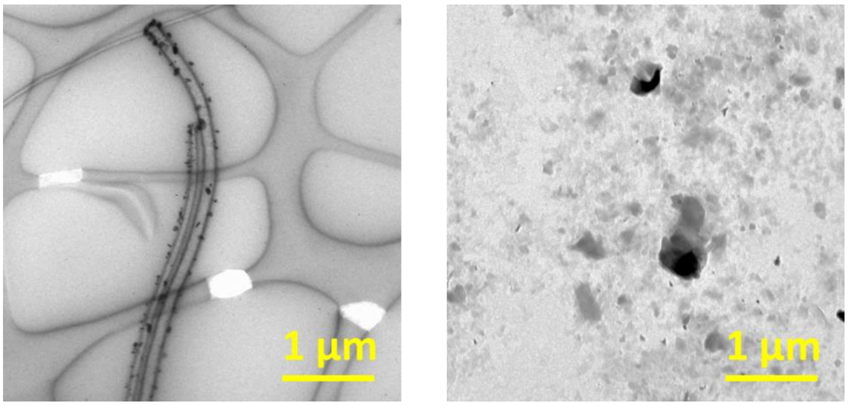

Fig. 1 TEM images of silver-decorated carbon nanofibers (left) and silver nanoparticles (synthesized without support)

Evaluating the rheological properties of the decontaminating formulations is critical when considering the application methods for treating contaminated surfaces (via spraying, brushing, rolling, etc.). All samples demonstrated a non-Newtonian pseudoplastic behavior, characterized by shear thinning behavior.

Further, the decontaminating formulations were crosslinked using a zinc acetate solution. These peelable coatings play a pivotal role in decontamination applications, as they must exhibit sufficient flexibility to be effortlessly peeled off as a continuous sheet once their purpose is fulfilled. All films obtained in this study exhibited mechanical properties suitable for facile peeling as a cohesive, uninterrupted sheet. The zinc acetate cross-linked hydrogels exhibited remarkable antimicrobial activity. These hydrogels rapidly create a sterile surface, effectively inactivating biological contaminants within 24 hours. Their decontamination efficiency against *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa* ranged from 96.8% to 99.95%. This high antimicrobial effect is attributed to the synergistic action of silver generated in the presence of the oxidized carbon nanofibers, combined with efficient entrapment of contaminants inside the peelable films.

Conclusions: These innovative formulations were remarkably effective at rapidly and thoroughly removing pathogens from contaminated sites.

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References:

[1] T. Capoun, J. Krykorkova, Comparison of Selected Methods for Individual Decontamination of Chemical Warfare Agents, Toxics, 2(2), 2014.

[2] Ellen Raber, Raymond McGuire, Oxidative decontamination of chemical and biological warfare agents using L-Gel, Journal of Hazardous Materials, 93(3), 339-352, 2002.

[3] G. Toader et. al., Peelable Alginate Films Reinforced by Carbon Nanofibers Decorated with Antimicrobial Nanoparticles for Immediate Biological Decontamination of Surfaces, Nanomaterials, 13(20), 2775, 2023.

SD-P13 SYNTHESIS AND CHARACTERIZATION OF ALGINATE/CHITOSAN-GRAPHENE OXIDE MATRICES IN NEUROGENERATION

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Abstract: *This article provides an insight in the utilization of chitosan (CS) /alginate (ALG)-graphene oxide (GO) composites in nerve regeneration. The use of CS and/or ALG matrices in nerve regeneration has been extensively investigated, and this approach has shown significant promise. Here we added GO to the CS/ALG matrices, due to its unique properties, which can enhance the performance of matrices in the context of nerve regeneration. In this study, we presented our research findings and advancements in this field, discussing the fabrication methods and characterization techniques.*

Key words: alginate; chitosan; neuro-regeneration; conductivity; SEM; FTIR

Introduction: The combined use of a CS or ALG scaffold with GO can facilitate nerve regeneration. GO can enhance electrical conduction, proving beneficial for nerve regeneration and for the development of scaffolds that support neuronal growth. The properties of GO can be advantageous in promoting synaptic development between neurons, thus contributing to nerve regeneration from anatomical but also functional point of view [1,2,3].

Experimental and/or Modelling: GO was prepared according to Hummer's method [4]. Sodium alginate was purchased from Fisher Scientific U.K. Ltd. Chitosan was purchased from Aldrich Sigma. Na_2HPO_4 and Na_3PO_4 were obtained from Reactivul București and glacial acetic acid pure from CHEMPUR. Glycerol was obtained from Honeywell. Phosphate-buffered saline (PBS) was obtained from Sigma Aldrich and Tween 80 from Sigma-Aldrich, Germany. Scanning Electron Microscopy (SEM); Spectroscopic Methods (UV-Vis Spectroscopy, FTIR); PL Spectrometry; Thermal Analysis (TG-DSC), Conductivity assessments were used for the complex evaluation of these materials.

Results and discussions: Characterizing CS and ALG scaffolds is crucial to ensure that they met specific requirements for nerve regeneration and to evaluate their effectiveness and performance. GO was successfully integrated into the ALG and CS matrices. As a consequence of the composition, an enhanced electrical conduction at higher concentrations of GO was observed. Furthermore, the matrices proved to have a good purity and homogeneity. Integration of GO into ALG or CS matrices led to alterations in surface morphology compared to pure ALG or CS scaffolds. Also, integration of GO into the matrices led to enhanced thermal stability of the resulting scaffold.

Conclusions: The ALG-GO and CS-GO films were effectively produced and described in this study. Valuable insights into the structural characteristics of the ALG-GO, CS-GO composite films were obtained, assessing their compatibility and electric responsive nature which are essential in nerve graftings.

References:

[1] Abdelbasset, W.K.; et al. Alginate-based hydrogels and tubes, as biological macromolecule-based platforms for Peripheral Nerve Tissue Engineering: A Review. *Annals of Biomedical Engineering* **2022**, *50*, 628–653.

[2] Ojeda-Hernández, D. D.; et al. Potential of Chitosan and Its Derivatives for Biomedical Applications in the Central Nervous System. *Front. Bioeng. Biotechnol.* **2020**, *8*, 389.

[3] Yang, B.; et al. Graphene oxide-composited chitosan scaffold contributes to functional recovery of injured spinal cord in rats. *Neural Regen Res.* **2021**, *16*, 1829-1835.

[4] Croitoru, A.; Oprea, O.; Nicoara, A.; Trusca, R.; Radu, M.; Neacsu, I.; Ficai, D.; Ficai., A.; Andronescu E. Multifunctional platforms based on graphene oxide and natural products. *Medicina* **2019**, *55*, 230.

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