EMEC 24

26th - 29th Nov 2024
Alicante, Spain

26th-29th November 2024
Alicante (Spain)

24th European Meeting on Environmental Chemistry

Organized by

Universitat d'Alacant
Universidad de Alicante

ASSOCIATION OF CHEMISTRY AND THE ENVIRONMENT

BOOK OF ABSTRACTS

24th European Meeting on Environmental Chemistry

Book of abstracts

26th-29th November 2024
Alicante (Spain)

Title

Book of abstracts - 24th European Meeting on Environmental Chemistry

Editors

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Book of abstracts

Date

November 2024

24th European Meeting on Environmental Chemistry

https://emec24.es/
Alicante (Spain)
26th-29th November 2024

BOOK OF ABSTRACTS

Conference Chairwoman:
Lorena Vidal

Conference co-Chairman:
Antonio Canals

Organized by
University of Alicante and Association of Chemistry and the Environment

Supported by

- Generalitat Valenciana - Conselleria d'Educació, Cultura, Universitats i Ocupació
- The Prince Sultan Bin Abdulaziz International Prize for Water
- EuChemS-DAC Sample Preparation Study Group and Network
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PREFACE

On behalf of the Organizing Committee, it is an honour and a pleasure to welcome you to the 24th European Meeting on Environmental Chemistry (EMEC24).

The EMEC is organized annually on behalf of the Association of Chemistry and the Environment (ACE). It traditionally comprises a wide range of topics in the field of environmental chemistry and interdisciplinary presentations are very welcome. The EMEC meeting always attracts high quality scientific presentations, plenary and keynote talks from internationally renowned researchers working in environmental chemistry and related fields.

The Department of Analytical Chemistry, Nutrition and Food Science and the University Institute of Materials of the University of Alicante are pleased to host the 24th European Meeting on Environmental Chemistry, which will be held in Alicante (Spain) from 26th to 29th November 2024.

The conference consists of a three-day meeting involving a total of 204 contributions. The scientific schedule comprises 2 Plenary Lectures, 7 Keynote Lectures, 25 Lectures, 25 Young Lectures, and 4 Lectures given by companies specialized in this field, who sponsored the conference. Additionally, two poster sessions, and exhibitions bringing us up to date on the latest advances and trends in the field are a key part of the conference. It is important to highlight that 74 contributions (i.e, posters and oral lectures) are presented by young researchers, who represent the future of this scientific discipline.

The Prince Sultan Bin Abdulaziz International Prize for Water, The Royal Spanish Society of Chemistry-Alicante Territorial Section, The EuChemS-DAC Sample Preparation Study Group and Network, and, Agilent, Bruker and Restek are sponsoring awards for the two best oral communications and the ten best poster communications presented by young researchers. The Scientific Committee is in charge of selecting the winners on the basis of both scientific relevance and presentation quality.

The social events that round off the programme are designed to encourage informal discussion between participants, as well as allowing them to enjoy the delicious food and cultural and leisure activities that our city has to offer.

Our main objective is to attain the level of excellence seen at the previous EMEC meetings. We are therefore preparing for this important scientific event with great effort and dedication to ensure a first-class scientific programme presenting the latest research and trends in Environmental Chemistry.

We are confident that the EMEC meeting will provide a broad forum for people from academia, research and industry to exchange ideas on the latest advances in research and development in environmental chemistry and technology.

We sincerely hope that you will be able to attend and participate, and we trust that this event will be of the highest scientific and human value, full of content, vibrancy and participation, fulfilling your every expectation.

We look forward to seeing you all in Alicante.

Antonio Canals

Lorena Vidal

Chairs of the 24th European Meeting on Environmental Chemistry (EMEC24)

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GENERAL INFORMATION

Conference address: **Carretera de San Vicente del Raspeig, s/n – 03690 San Vicente del Raspeig, Alicante (ES)**

Conference web site: https://emec24.es/

Poster communications

There are two poster sessions scheduled in the Scientific Program:

- **POSTER SESSION I**: Wednesday, 27 November 2024 (16:00-17:00)
    - **AgroEnvironmentally Friendly Processes and Food Chemistry** (P-AgroEnv-01 - P-AgroEnv07) **and Young Poster** (PY-AgroEnv-01 - PY-AgroEnv-02)
    - **Climate Change: New Challenges** (P-ClimChange-01) **and Young Posters** (PY-ClimChange-01 - PY-ClimChange-03)
    - **Environmental Modelling** (P-EnvModel-01 - P-EnvModel-06)
    - **Environmental Monitoring** (P-EnvMonit-01 - P-EnvMonit-38) **and Young Posters** (PY-EnvMonit-01 - PY-EnvMonit13)
    - **Environmental Safety** (P-EnvSaf-01 - P-EnvSaf-04) **and Young Posters** (PY-EnvSaf-01 - PY-EnvSaf-05)
- **POSTER SESSION II**: Thursday, 28 November 2024 (17:10-18:00)
    - **Environmental Technologies** (P-EnvTech-01 - P-EnvTech-14) **and Young Posters** (PY-EnvTech-01 - PY-EnvTech-12)
    - **Green Chemistry and Green Technologies** (P-GreenChem-01 - P-GreenChem-14) **and Young Posters** (PY-GreenChem-01 - PY-GreenChem-10)
    - **Sustainable Development** (P-SustDev-01 - P-SustDev07) **and Young Posters** (PY-SustDev-01 - PY-SustDev-04)

Prince Sultan Bin Abdulaziz
International Prize for Water

Recognizing Innovation

Winners for the 11th Award (2024)

Creativity Prize

Creativity Prize

[1] The team of Maria Cristina Rulli (Polytechnic of Milan, Italy) and Paolo D'Odorico (University of California, Berkeley, USA)

for spearheading novel analyses of the water-energy-food nexus that describe how numerous complex factors interact, providing for better freshwater stewardship in a changing, globalised world.


Maria Cristina Rulli


Paolo D'Odorico

[2] The team of Zhiguo He (Zhejiang University, China)

for developing working, versatile soft robots with unprecedented manoeuvrability that have the capacity for numerous underwater research and monitoring applications. Team members include: Pengcheng Jiao and Yang Yang.


Zhiguo He

Surface Water Prize

Surface Water Prize

Qiuhua Liang (Loughborough University, UK) and his team

for developing innovative, open-source, multi-GPU hydrodynamic models to support real-time flood forecasting at high temporal-spatial resolutions. Team members include: Huili Chen, Xiaodong Ming, Xilin Xia, Yan Xiong and Jiaheng Zhao.


Qiuhua Liang

Groundwater Prize

Groundwater Prize

Chunmiao Zheng (EIT, Ningbo, China) and his team

for powerful modelling tools to understand groundwater processes and manage groundwater resources under diverse eco-hydrological and climatic conditions, considering environmental and socioeconomic factors at local and national scales.


Chunmiao Zheng

Alternative Water Resources Prize

Alternative Water Resources Prize

Virender K. Sharma (Texas A&M University, USA) and his team

for the effective removal of antibiotics and pharmaceuticals from wastewater through advanced oxidative processes by activated ferrate, which work at high, even enhanced, efficiency in water containing commonly occurring natural organic matter. Team members include: Ching-Hua Huang, Chetan Jinadatha and Radek Zbořil.


Virender K. Sharma

Water Management & Protection Prize

Water Management & Protection Prize

Joseph Hun-wei Lee (Macau University of Science & Technology, China)

for developing unique and highly effective hydro-environmental modelling systems for the sustainable water management of smart cities.


Joseph Hun-wei Lee

Invitation for Nominations

12th Award (2026)

Nominations open online until 31 December 2025

www.psipw.org e-mail: info@psipw.org

THE PROGRAMME AT A GLANCE

The programme schedule is given in CET

	Tuesday 26
18:00	**Welcome Cocktail & Music Concert**

	Wednesday 27
8:00	**Registration**
9:00	**Opening session**
10:00	**Oral Session 1** Environ. Monit. I & Climat. Change
11:00	**Coffee & Exhibition**
11:30	**Oral Session 2** Environ. Monit. II
13:00	**Lunch**
14:30	**Oral Session 3** Environ. Monit. III
16:00	**Poster Session 1**
17:00	**Guided tour** **ECR workshop**

	Thursday 28
8:00	**Registration**
9:00	**Oral Session 4** Environ. Monit. IV
10:00	**Oral Session 5** Agro-Environ. & Environ. Modelling
11:00	**Coffee & Exhibition**
11:30	**Oral Session 6** Environ. Monit. V & Sust. Dev. & Green Chem.
13:00	**Lunch**
14:30	**Oral Session 7: Young Session I** (Auditorium) **Oral Session 8: Young Session II** (Classroom)
15:30	**Coffee & Exhibition**
16:00	**Oral Session 9: Young Session III** (Auditorium) **Oral Session 10: Young Session IV** (Classroom)
17:10	**Poster Session 2**
20:00	**Gala dinner**

	Friday 29
9:00	**Oral Session 11** Environ. Monit. VI & Technol. & Safety
10:35	**Coffee & Exhibition**
11:30	**Oral Session 12** Environmental Technol.
12:30	**ACE GENERAL ASSEMBLY**
13:00	**Brunch**
14:00	**Closing session**

SCIENTIFIC PROGRAMME OF EMEC 2024

The programme schedule is given in CET

Tuesday, 26th November 2024

18:00-20:00	**Welcome Cocktail & Music Concert (Museum of the University of Alicante, MUA)**

Wednesday, 27th November 2024

8:00-9:00		REGISTRATION
9:00-10:00		OPENING SESSION
9:00-9:20		Opening ceremony
9:20-10:00	PL-01	**Climate change and air pollution: two silent killers** Pedro Jiménez-Guerrero

Oral Session 1: Environmental Monitoring I & Climate Change
Chairs: Branimir Jovančićević and Malgorzata Iwona Szynkowska-Jozwik

10:00-10:20	KN-01	**Birds as biomonitors of environmental pollution** Silvia Lacorte, B. Oro-Nolla, M. Dulsat-Masvidal, F. J. Santos, A. Bertolero
10:20-10:40	KN-02	**Polycyclic aromatic compounds – atmospheric fate and environmental exposure** Gerhard Lammel
10:40-10:55	O-01	**Advances in the electrochemical reduction of CO_2 into formate/formic acid** Jose Solla-Gullón, E. Bujedo-Saiz, B. Ávila-Bolívar, A. Peña-Rodríguez, K. Fernández-Caso, M. Molera, G. Díaz-Sainz, A. Irabien, V. Montiel, T. Andreu, M. Alvarez-Guerra, J. Albo, J. Iniesta
11:00-11:30		COFFEE & EXHIBITION

Oral Session 2: Environmental Monitoring II
Chairs: Jesús Iniesta and Maja Turk

11:30-11:45	O-02	**Semi-volatile organic pollutants in the Polar Arctic atmosphere: Long-term passive sampling and GC-HRMS analysis** Albert T. Lebedev, I.S. Shavrina, D.S. Kosyakov
11:45-12:00	O-03	**Bioaccumulation, organotropism and toxicological risk of trace elements in Caretta caretta (Linnaeus, 1758)** Dario Savoca
12:00-12:15	O-04	**Biodegradation of bisphenol A and its analogues by green algae and cyanobacteria** Karolina Czarny-Krzymińska, B. Krawczyk, D. Szczukocki
12:15-12:30	O-05	**Ceramic passive samplers for the analysis of organic contaminants in water** Evgeny Bulatov, J. Silva, M. Laguna, E. Vazquez, S. Lacorte

12:30-12:45	O-06	**Combining waste PET-MIL-101(Fe) and cellulose acetate polymeric membrane for the preconcentration and extraction of neonicotinoid insecticides in water samples** Philiswa Nosizo Nomngongoa, S. Jakavula
12:45-13:00	O-07	**Application of passive samplers for the evaluation of trace metals in the Llobregat River basin, Spain** Marta Turull, S. Valdivielso, D. Jurado, J. Botey, E. Vázquez-Suñé, S. Carrero, C. Fontàs, S. Díez
13:00-14:30		LUNCH

Oral Session 3: Environmental Monitoring III
Chairs: Albert T. Lebedev and Polonca Trebše

14:30-14:50	OS-01	**Latest trends in PFAS testing and regulations landscape** Emanuele Ceccon, M. Chang
14:50-15:10	OS-02	**Enhancing non-targeted analysis using comprehensive-two-dimensional gas chromatography coupled to a high-resolution mass spectrometry in environmental samples** Julio Lluch, S. Pantó, D. Rakov, A. Khalefa, N. Jones
15:10-15:25	O-08	**Impact of agricultural emissions on rural and urban air quality (IMAGE)** Vivien Corona, D. O'Connor, S. Hellebust, A. Gilmer, V. Byers, A. Donnelly, E. McGillicuddy
15:25-15:40	O-09	**LC-HRMS response to the mystery of nano/microplastics: A study focused on detection and identification of plastic polymers and their photooxidation products** Raghav Dogra, L. Carena, D. Fabbri, D. Vione, M. Passananti
15:40-15:55	O-10	**Ozone (O_3) trends in Saxony (Germany) and insights from photochemical modelling** Yaru Wang, D. van Pinxteren, A. Tilgner, E.H. Hoffmann, L. Poulain, M. Hell, S. Bastian, H. Herrmann

16:00-17:00 POSTER SESSION 1 & COFFEE & EXHIBITION

17:00-19:00 **Guided tour**

17:00-20:00 **ECR workshop** (Auditorium)
Early-career research workshop: *Hunting for a postdoc that's right for you – Tips & Resources*

17:00-18:30	Workshop with speakers and interactive panel discussion
18:30-20:00	Catered networking & social session

Thursday, 28th November 2024

Oral Session 4: Environmental Monitoring IV
Chairs: María Llompart and Miguel Ángel Aguirre

9:00-9:20	KN-03	**Are we aware of the role of enantioselectivity in the environment?** Ana Rita Lado
9:20-9:40	KN-04	**Suspect and non-target screening of persistent organic pollutants in environmental samples by two-dimensional gas chromatography–time-of-flight mass spectrometry** Lourdes Ramos
9:40-10:00	KN-05	**Organic UV filters as indicators of antropogenic micropollution in insular ecosystems** José Juan Santana, M.I. Cadena-Aizaga, S. Montesdeoca-Esponda, Z. Sosa-Ferrera

Oral Session 5: Agro-Environmentally Friendly Processes and Food Chemistry & Environmental Modelling
Chairs: Alfonso Jiménez and Jelena Radonić

10:00-10:15	O-11	**Valorization strategies of plants and algae alien invasive species: new developments contributing to the circular economy** María del Carmen Garrigós, R. Niamet Allah Belhadj, C. Mellinas, C. Bordehore, A. Jiménez
10:15-10:30	O-12	**Development of active packaging based on activated carbon obtained from biomass waste to extend the shelf life of fruits** Jessica Chaparro-Garnica, N. Ortuño, T. Calvo, J. Palenzuela, E. Morallón, D. Cazorla-Amorós
10:30-10:45	O-13	**Environmental risk modelling of pharmaceuticals in the water environment: Towards eco-directed prescribing in Scotland** Lydia Niemi, N. Arakawa, M. Glendell, Z. Gagkas, S. Gibb, C. Anderson, S. Pfleger
10:45-11:00	O-14	**Photoinduced mineralisation of organic matter in the global lakes** Davide Vione, L. Carena, Á. García Gil, J. Marugán
11:00-11:30		COFFEE & EXHIBITION

Oral Session 6: Environmental Monitoring V & Sustainable Development & Green Chemistry
Chairs: Elefteria Psillakis and José Juan Santana

11:30-11:45	O-15	**The need of analysis of new substances in drinking and bottled waters** Rajmund Michalski
11:45-12:00	O-16	**Environmental emergencies: nanoplastics and microplastics, impacts and solutions** Reda Dzingelevičienė, N. Dzingelevičius, S. Abbasi, V. Abromaitis, R. Vaičekauskaitė, A. Razbadauskas, B. Buszewski
12:00-12:15	O-17	**Modern smoking – vaping – inhalation of other volatile organic compounds (VOCs) besides nicotine** Mojca Bavcon Kralj, T. Kocmut, B. Poljšak, P. Trebše
12:15-12:30	O-18	**Synthesis, evaluation of halogenated BPA and paraben compounds** Pascal Carato, M. Grimaldi, C. Tomkiewicz, L. Larigot, S. Leneuf de Neufville, E. Bourdeaud, M. Thomas, P. Balaguer, X. Coumoul

12:30-12:45	O-19	**Isolation of cellulose from soybean hulls: efficiency and sustainability of different strategies** Maria Laura Tummino, M. Rigoletto, G. Grillo, E. Natali, E. Laurenti, S. Tabasso
12:45-13:00	O-20	**MICROPLASTICS from tires. An emerging concern** María Llompart, A. Duque-Villaverde, S. Sóñora, V. Carballeira, N. Montero, D. Armada, P. Nurerk, T. Dagnac
13:00-14:30		LUNCH

Oral Session 7. YOUNG RESEARCHERS I: Green Chemistry & Green Technologies
Chairs: Silvia Lacorte and Nuno Ratola

Auditorium

14:30-14:40	OY-01	**Bifunctional carbon-supported Pd-based catalysts for the sustainable production and storage of H_2 attained by formic acid-bicarbonate couple** Paula Riquelme-García, M. Navlani-García, D. Cazorla-Amorós
14:40-14:50	OY-02	**Biotechnological valorisation of acid mine drainage: Seaweed as a green tool for rare earth elements recovery** Thainara Viana, N. Ferreira, E. Pereira, B. Henriques
14:50-15:00	OY-03	**Bisphenols extraction from water samples employing a natural deep eutectic solvent-based liquid-liquid microextraction technique** Iván Rubio, J. Rayos, I. Ortega, M.Á. Aguirre, L. Vidal, A. Canals
15:00-15:10	OY-04	**Chitosan, gelatine and cellulose based hydrogels for the removal of potentially toxic elements from aquaculture water: a comparative study** Monica Rigoletto, M. Malandrino, S. Berto, P. Calza, E. Laurenti, M. Sangermano, R. Sesia
15:10-15:20	OY-05	**Innovative electrochemically controlled liquid-liquid microextraction (EC-LLME) using hydrophilic deep eutectic solvent for efficient heavy metal extraction from edible oil samples** Andrea Marco, B. Pertusa, C. Quijada, M.Á. Aguirre, M. Hidalgo
15:20-15:30	OY-06	**Sheath flow chemistry for 4D-Architecture of necklaced fertiliser: minimising agrochemical leachate** Tu Nguyen Quang Le, C. Lim, I. Fisk, N. Nghiep Tran, V. Hessel, K. Robertson

Oral Session 8. YOUNG RESEARCHERS II: Miscellaneous: Agro-environmentally Friendly Processes & Climate Change & Sustainable Development and Environmental Technologies
Chairs: Manuel Miró and Lourdes Ramos

Classroom: A2/E13

14:30-14:40	OY-07	**Immobilization of Burkholderia cepacia lipase on eggshell membrane-based carriers** Marta Ostojčić, M. Stjepanović, I. Strelec, S. Budžaki
14:40-14:50	OY-08	**Can a laboratory predict the field?** Nevena Antić, M. Kašanin-Grubin, B. Jovančićević
14:50-15:00	OY-09	**Evaluating sustainability of direct aptamer assays for the nucleocapsid protein of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2)** Ana García-Juan, R. Serrano, G. Grindlay, L. Gras, J. Mora
15:00-15:10	OY-10	**Structural features and health effects of water-soluble organic matter from atmospheric fine air particulates** Antoine S. Almeida, B.M. Neves, R.M. B. O. Duarte

15:10-15:20	OY-11	**Sustainable and environmentally friendly processes to synthesise highly stable N-doped activated carbons** Jorge Sánchez Carrasco, J. Chaparro-Garnica, D. Salinas-Torres, E. Morallón, D. Cazorla-Amorós
15:20-15:30	OY-12	**Bioremediation of industrial brines using Haloferax mediterranei R4: the specific case of wastewater coming from a desalination plant, a textile industry, and an olive production company** Iraide Sáez-Zamacona, R.M. Martínez-Espinosa, G. Grindlay
15:30-16:00		COFFEE & EXHIBITION

Oral Session 9. YOUNG RESEARCHERS III: Environmental Monitoring
Chairs: Silvia Lacorte and Nuno Ratola

Auditorium

16:00-16:10	OY-13	**Detection of persistent, mobile and toxic contaminants in aqueous matrices by high performance liquid chromatography and mass spectrometry** Sandra Méndez, M. Perin, R. Rodil, L. Bijlsma, E. Pitarch, V. Acuña, J. Comas, R. Montes, J.B. Quintana
16:10-16:20	OY-14	**Electrochemical determination of acetylcholinesterase activity for evaluating ecotoxicological threats in marine environments** Salma Hafed-Khatiri, D. Salinas-Torres, F. Montilla
16:20-16:30	OY-15	**Optimizing the recovery of Rare Earth elements from aqueous mediums using easily separated manganese ferrites** João Pinto, D. Tavares, B. Henriques, R. Fernandes, T. Trindade, E. Pereira
16:30-16:40	OY-16	**Portable cost-effective colorimetric detection of polycyclic aromatic hydrocarbons using an iPhone 11 camera** Caoilte O'Rourke O'Cuirrin, F. Regan, M. Vázquez
16:40-16:50	OY-17	**Study of PFAS contamination in drinking waters of the Fos-Berre area (France)** Maëlys Dijoux, A. Piram, S. Augy, A. Austruy, A. Souloumiac, E. Gonzales-Camoin, J. Dron, X. Moreau, L. De Jong, T. Orsière, S. Gori, P. Wong-Wah-Chung, P. Doumenq
16:50-17:00	OY-18	**Understanding the degradation of bio-based polymers across contrasting marine environments** Alba Benito-Kaesbach, A. Beltrán-Sanahuja, N. Casado-Coy, R. T. Mathers, C. Sanz-Lázaro

Oral Session 10. YOUNG RESEARCHERS IV: Environmental Technologies
Chairs: Manuel Miró and Lourdes Ramos

Classroom: A2/E13

16:00-16:10	OY-19	**Emerging organic contaminants degradation and faecal bacteria indicators elimination by a new filterless domestic purification system** Ian Vedeau, S. Lebarillier, M. Willkomm, A.-M. Farnet Da Silva, P. Wong Wah Chung
16:10-16:20	OY-20	**Energy-efficient UASB de-ammonification for wastewater management** Divyesh Parde, M. Behera, R. Roshan Dash
16:20-16:30	OY-21	**Enhancing microbial electrosynthesis with polyaniline as cathode catalyst for CO_2 capture and conversion to green chemicals** Rahul Ghosh, M. Behera
16:30-16:40	OY-22	**Investigation of sorption and photochemical capacity of sewage sludge derived biochar for the removal of water contaminants** Marina Anastasiou, V. Sakkas, M. Sleiman

16:40-16:50	OY-23	**Study and modelization of an electrodialysis process for saline wastewater regeneration and reuse in agriculture** Vicent Ayala-Andreu, M.Á. Montiel López, V. García-García, J. Antonio Labarta Reyes, F. Etchebarne, F. Lutin, V. Montiel Leguey
16:50-17:00	OY-24	**Titanium dioxide – Carbon Dots nanocomposites for the visible-light and sunlight-driven photodegradation of organic pollutants** Ricardo Sendão, J. Esteves da Silva, L. Pinto da Silva
17:00-17:10	OY-25	**Unravelling UV-induced photochemical mechanisms for nano-polystyrene removal from water** Yongrong Zou, H. Clermont, G. Mailhot, M. Sleiman

17:10-18:00 POSTER SESSION 2

20:00 GALA DINNER

Friday, 29th November 2024

Oral Session 11: Environmental Monitoring VI & Environmental Technologies & Environmental Safety

Chairs: Gerhard Lammel and Ana Rita Lado

9:00-9:20	KN-06	**Biochemicall strategies for valorisation of agrifood side streams for a circular primary sector** Francisco Javier Vilaplana
9:20-9:40	KN-07	**Physiologically-based extraction assays of plasticizers from microplastics: Is the 'Trojan-horse' effect hype or reality?** Manuel Miró, A. Sixto, J. López-Vázquez, J. Benito Quintana, R. Rodil
9:40-10:00	OS-03	**Accurate microplastics characterization on water samples with aluminum-coated filters using QCL IR chemical imaging** Fernando Tobalina, D. Robey, T. Kumanayaka, A. Kerstan, W. Alwan
10:00-10:20	OS-04	**From known to unknown in mass spectrometry: an example with PFAS challenge in environmental samples** Pedro Cano, M.A. Pérez, J. Gómez-Espina, E. Bueno
10:20-10:35	O-21	**Electrochemical monitoring of BIT photo(catalytic)degradation** Polonca Trebše, Ł. Szkudlarek, M. Bavcon Kralj, A. Šuligoj, M. Hadolin, N. Sodnik, K. Soderžnik Žagar
10:35-11:30		COFFEE & EXHIBITION

Oral Session 12: Environmental Technologies

Chairs: Francisco Javier Vilaplana and Jan Schwarzbauer

11:30-11:45	O-22	**PFAS removal by minerals and advanced removal by tailored polymer-mineral composites** Yael Mishael, H. Menuchin, M. Samara, A. Nasser
11:45-12:00	O-23	**Resource recovery from wastewater with biochar: quality assessment and phosphorus fractionation** Sabolc Pap, T. Thompson, C. Karmann, T. Kennedy, R. McNeil, S.W. Gibb, M. A. Taggart[a]
12:00-12:15	O-24	**Promoting the self-immobilisation of activated carbon for enhanced adsorption of organic micropollutants** André Torres-Pinto, J.J.M. Dele, A.M. Chávez, A.M.T. Silva
12:15-12:30	O-25	**Heavy metals levels in the close neighbourhood of the industrial waste landfills in Lodz region** Aleksandra Pawlaczyk, M. Smarzyk, M. Zaborowski, D. Kryszczak, M.I. Szynkowska-Jóźwikik
12:30-13:00		**ACE GENERAL ASSEMBLY**
13:00-14:00		BRUNCH
14:00-15:00		CLOSING SESSION
14:00-14:40	PL-02	**Cigarette waste leachates: an overlooked environmental issue** Elefteria Psillakis
14:40-15:00		Closing Ceremony & Awards

POSTER SESSIONS

POSTER SESSION 1: Wednesday 27th, 16:00-17:00

AGRO-ENVIRONMENTALLY FRIENDLY PROCESSES AND FOOD CHEMISTRY

P-AgroEnv-01	**From the soil to the wine – elements' migration in monovarietal Bulgarian wines** Elisaveta Mladenova, Tsvetomil Voyslavov
P-AgroEnv-02	**Application of hydrolytic enzymes for the removal of fats and oils from wastewater** Marija Stjepanović, Natalija Velić, Marta Ostojčić, Nikola Maravić, Zita Šereš, Sandra Budžaki
P-AgroEnv-03	**Thermal processing effect on element absorption from honey bee (*Apis mellifera*) feed** Nenad M. Zarić, Walter Goessler, Slobodan Dolašević, Miloš Petrović, Ratko Pavlović
P-AgroEnv-04	**Optimization of a sensitive methodology based on ultrasound-assisted extraction emulsification microextraction (USAEME) and high-resolution mass spectrometry for the analysis of multi class herbicides in water** Thierry Dagnac, Sergio Sóñora, Ana Castiñeira-Landeira, Maria Llompart
P-AgroEnv-05	**Brewers' spent grain and wild edible herbs as starting material for new functional confectionery products** Vesna Antić, Nebojša Pantelić, Milica Balaban, Dajana Janjušević, Jelena Isailović, Margarita Dodevska, Snežana Zlatanović, Mališa Antić, Milica Stevanović, Jovanka Laličić-Petronijević
P-AgroEnv-06	**Biological effectiveness of newly synthesized $[NiL\ (H_2O)_2]$ on fungy *Phomopsis viticola*** A. Radović, Željko Jaćimović, Bogoljub Kandić, N. Latinović, Miljan Bigović
P-AgroEnv-07	**Valorization of lignocellulosic residues generated in the Valencian Community for environmental applications. The NIRALIG project** Alfonso Jiménez, Carlos Pelegrín, María del Carmen Garrigós

YOUNG POSTER

PY-AgroEnv-01	**Investigation of deep eutectic solvent-modified oat straw as an efficient adsorbent for Zn(II) ion removal: structural and kinetic study** Jelena Dimitrijević, Sanja Jevtić, Marija Simić, Marija Koprivica, Aleksandar Marinković, Marija Ercegović, Jelena Petrović
PY-AgroEnv-02	**Comprehensive studies on cadmium removal in the phosphate fertilizer industry through the adsorption process** Urszula Ryszko, Dorota Kołodyńska

CLIMATE CHANGE: NEW CHALLENGES

P-ClimChange-01	**Facile hydrothermal synthesis of $g\text{-}C_3N_4/Cu_3TeO_6$ heterostructure with H_2 production photocatalytic properties** Javier Fernández-Catalá, Jonny Chávez-Caiza, Rossella Greco, Miriam Navlani-García, Wei Cao, Ángel Berenguer-Murcia, Diego Cazorla-Amorós

YOUNG POSTERS

PY-ClimChange-01	**Effects of nitrated monoaromatic hydrocarbons from biomass burning aerosols on chemical composition of the marine microalgae *Dunaliella tertiolecta*** Saranda Bakija Alempijević, Sanja Frka, Blaženka Gašparović, Slađana Strmečki
PY-ClimChange-02	**From classroom to consciousness: a hands-on approach to waste management for young students** Slađana Savić, Nebojša Radović, Željka Nikolić, Olga Tešović, Ksenija Stojanović
PY-ClimChange-03	**High activity Pd/carbon catalysts prepared from biomass residues for hydrogen production and storage** María Bernal-Vela, Miriam Navlani-García, Diego Cazorla-Amorós

ENVIRONMENTAL MODELLING

P-EnvModel-01	**Morphological analysis of microplastics revisited – application of pattern recognition and computer vision tools** Aleksander Astel, Paulina Piskuła
P-EnvModel-02	**Investigation of the effect of sulfates in Fenton reactions in aerosol conditions** Daniele Scheres Firak, Thomas Schaefer, Celine Kula, Hartmut Herrmann
P-EnvModel-03	**Seasonal $PM_{2.5}$ land use regression models for Novi Sad, Serbia** Sonja Dmitrašinović, Jelena Radonić, Milena Jovašević Stojanović, Miloš Davidović
P-EnvModel-04	**Occurrence, dissipation kinetics and environmental risk assessment of antibiotics and their metabolites in agricultural soils** Carmen Mejías, Laura Martín-Pozo, Marina Arenas, Juan Luis Santos, Julia Martín, Irene Aparicio, Esteban Alonso
P-EnvModel-05	**Dissipation of endocrine disrupting chemicals in soil: impact of microplastic contamination** Laura Martín-Pozo, Carmen Mejías, Juan Luis Santos, Julia Martín, Irene Aparicio, Esteban Alonso
P-EnvModel-06	**Microalgae meeting with therapeutic muds: the change in organic matter contents and *n*-alkane distributions as a fingerprint for peloid's microalgal enrichment** Nikola Burazer, Anđela Sekulović, Gorica Veselinović, Urška Šunta, Aleksandra Šajnović, Branimir Jovančićević

ENVIRONMENTAL MONITORING

P-EnvMonit-01	**Analysis of the total mercury content in soil samples from the city of Lodz in central Poland** Elżbieta Maćkiewicz, Małgorzata Furmanek, Małgorzata Iwona Szynkowska-Jóźwik
P-EnvMonit-02	**Mercury in air and environmental samples near Europe's largest lignite-fired power plant** Elżbieta Maćkiewicz, Małgorzata Iwona Szynkowska-Jóźwik
P-EnvMonit-03	**Geochemical dynamics and risk assessment of potentially toxic metals in irrigated agricultural soils of the Mediterranean region** Mariana Custódio, Adriana Catarino, Alexandra Tomaz, José Dôres, Manuel Patanita, Patricia Palma
P-EnvMonit-04	**Understanding the sources of marine litter in remote islands: the Galapagos islands as a case study** Alba Benito-Kaesbach, Jenifer Suárez-Moncada, Alfonso Velastegui, Jerson Moreno-Mendoza, Mariana Vera-Zambrano, Ulises Avendaño, Peter G. Ryan, Carlos Sanz-Lázaro
P-EnvMonit-05	**Aqueous ozonolysis of the antiviral drug Umifenovir (Arbidol)** Albert T. Lebedev, Sergey A. Sypalov, Ilya S. Varsegov, Elena.V. Danilova, Nikolay.V. Ul'yanovskii, Dimitry S. Kosyakov
P-EnvMonit-06	**Environmental monitoring in the Italian seas by means of descriptor 8 of marine strategy framework directive** Chiara Maggi, Maria Teresa Berducci, Paola Guarracino, Giulia Fucile, Manuela Dattolo, Antonella Cozzolino, Giulio Sesta, Anna Lauria, Lorenzo Lusco, Giulia Romanelli, Marina Amici, Roberta Parravano, Valerio Fabrizi, Luca Trigilio, Valentino Perini, Giuseppina Ciuffa, Andrea Colasanti
P-EnvMonit-07	**Biomonitoring phthalic acid esters in marine turtles: sources of contamination and potential implications** Dario Savoca
P-EnvMonit-08	**Impact of organic contaminants in soils from important bird and biodiversity areas** Maria Dulsat-Masvidal, Carlos Ciudad, Octavio Infante, Rafael Mateo, Silvia Lacorte
P-EnvMonit-09	**Assessing contamination profiles in livers from road-killed owls** Maria Dulsat-Masvidal, Rui Lourenço, Rafael Mateo, Silvia Lacorte
P-EnvMonit-10	**Evaluating an invasive bivalve as a potential environmental proxy for metals in a large South American basin** Esteban Avigliano, Jorge Pisonero, Ana Méndez, Cristhian Clavijo, Pablo Scarabotti, Jacqueline Caffetti, Juan F. Facetti
P-EnvMonit-11	**The evolving landscape of PFAS detection, an outline of methods** Fernando Rodríguez Carrero, Jamie York, Shun-Hsin Liang, Tina Brandscher, Sandra Ruiz Perez
P-EnvMonit-12	**A hybrid stationary phase of ion-exchange and hydrophilic interaction chromatography for the LC/MS of polar compounds** Fernando Rodríguez Carrero, Diego López, Shun-Hsin Liang, Xiaoning Lu
P-EnvMonit-13	**Integrated chemical and biological methods for studying the neurotoxic effects of air pollution: application to air samples from Catalonia** Esmeralda Ayala, Barend L. van Drooge, Carmen Bedia
P-EnvMonit-14	**Relationship between total phosphorus, salinity and dissolved oxygen, with *chlorophyll a* in Lagos coastal waters; implication on seasonal eutrophication** Folake O. Echebiri, Najeem O. Oladosu, Akeem A. Abayomi, Kehinde O. Olayinka, Babajide I. Alo

P-EnvMonit-15	**Enantioselective degradation of chiral β-blockers in soil treated with sewage sludge and irrigated with wastewater** Marina Arenas, Noelia García-Criado, Julia Martín, Juan Luis Santos, Irene Aparicio, Esteban Alonso
P-EnvMonit-16	**Matrix solid-phase dispersion for determination of tetracyclines in solid environmental samples** Noelia García-Criado, Marina Arenas, Julia Martín, Juan Luis Santos, Irene Aparicio, Esteban Alonso
P-EnvMonit-17	**Employing cutting-edge methodologies for in-depth spatiotemporal analysis of water quality dynamics in Serbian rivers** Maja Brborić, Sonja Dmitrašinović, Sanja Ćojbašić, Maja Turk Sekulić, Jelena Radonić
P-EnvMonit-18	**Implementation plan to monitor microplastics in surface and drinking water according to Directive (EU) 2020/2184: Barcelona case study** Joan Dalmau-Soler, M. Rosa Boleda, Sílvia Lacorte
P-EnvMonit-19	**Health risk assessment of rare earth elements in road dust near coal-fired thermal power plants** Jovana Roganović, Dubravka Relić, Milana Zarić, Mira Aničić Urošević, Inga Zinicovscaia, Konstantin Ilijević, Nenad Zarić
P-EnvMonit-20	**Selenium speciation in the aqueous samples of old Salsigne mining area (Aude, France)** Lucija Knezevic, Sophie Delpoux, Rémi Freydier, Benoit Madé, Philippe Behra, Corinne Casiot
P-EnvMonit-21	**Mineral composition of soil as an indicator of the geographical origin of single-varietal wines** Małgorzata Iwona Szynkowska-Jozwik, Magdalena Gajek, Weronika Olejniczak, Piotr Wysocki, Aleksandra Pawlaczyk
P-EnvMonit-22	**Monitoring of trace element levels in soil from areas surrounding highways and expressways in the Lodz region in Poland** Małgorzata Iwona Szynkowska-Jozwik, Damian Kryszczak, Małgorzata Szczesio, Aleksandra Pawlaczyk, Jadwiga Albinska
P-EnvMonit-23	**Hydrochemical and isotopic characterization of the waters in the upper basins of the Llobregat and Cardener Rivers** Sonia Valdivielso, Deby Juraro, Marta Turull, Joan Botey, Sergio Carrero, Sergi Díez
P-EnvMonit-24	**Electrochemical biosensing of alkaline phosphatase inhibitors** María J. Sáenz-Espinar, Francisco Huerta, Francisco Montilla
P-EnvMonit-25	**Preconcentration of selected cephalosporins using waste pet-derived UIO-66 as an adsorbent before HPLC-DAD quantification** Mthokozisi Mnguni, Andisiwe Bangani, Philiswa Nosizo Nomngongo
P-EnvMonit-26	**Can SVOC levels in pine needles from different species be comparable?** Nuno Ratola, Sofia Augusto, Zulema Varela, Marzieh Moeenfard, José Avelino Silva, Sara Ramos, Francisco Cereceda-Balic, Ximena Fadic, Marius Matache
P-EnvMonit-27	**Comparing elemental composition of bumblebees to honey bees as biomonitors of metals** Nenad M. Zarić, Lena Benner
P-EnvMonit-28	**INCOME – Inputs for a more sustainable region: Tools for managing metal-contaminated areas** Mariana Custódio, Rui J. Oliveira, Ana Fialho, B. Caldeira, Maria J. Costa, Patricia Palma
P-EnvMonit-29	**Co-dispersion of 3,3’,5,5’-tetramethylbenzidine and nanocellulose in water leads to durable iron(III)-responsive suspensions** Roberto J. Aguado, Núria Fiol, Quim Tarrés, Marc Delgado-Aguilar

P-EnvMonit-30

PAH Profiles of emitted smoke from burley tobacco stalk briquettes and its combinations with other types of biomass
Sanja Stojadinović, Maja Malnar, Gorica Veselinović, Snežana Štrbac, Lazar Pejić, Vesna Radojičić

P-EnvMonit-31

Canopy density for tree species in an urban park
Snežana Štrbac, Sanja Stojadinović, Nevena Antić, Nikola Živanović, Vukašin Rončević, Milica Kašanin-Grubin,

P-EnvMonit-32

Development and improvement of high throughput methods for the determination of emerging pollutants included in the European legislation on water policy
Iago Riveiro, Javier López-Vázquez, Rosa Montes, José Benito Quintana, Rosario Rodil

P-EnvMonit-33

Development of an enzymatic biosensor for the detection of environmental stress markers in coral species via glutathione S-transferase reactions
Catalina Farcas, Francisco Montilla

P-EnvMonit-34

Analytical methodology for the determination of pharmaceuticals and other emerging contaminants used as indicators of the quaternary treatment of urban wastewater
Andres Duque-Villaverde, Sergio Sóñora, Raissa Antonelli, Vítor J.P. Vilar, Thierry Dagnac, Maria Llompart

P-EnvMonit-35

Assessment of the level of self-cleaning of the soils around the former metallurgical plant – Kremikovtsi, Bulgaria
Tsvetomil Voyslavov, Elisaveta Mladenova, Stela Georgieva

P-EnvMonit-36

The presence of plastic pollution in the biosphere reserve of the Tara River Basin
Neda Bošković, Željko Jaćimović

P-EnvMonit-37

Methods for fluorine determination in raw material for gasoline blending
Zofia Kowalewska

P-EnvMonit-38

Field validation of a novel passive air sampler – monitoring of semivolatile organic pollutants in the remote marine and continental boundary layer
Gerhard Lammel, Björn Nillius, Frank Helleis, Adela Holubová Šmejkalová, Petr Kukučka, Jakub Martiník, Petra Přibylová, Roman Prokeš, Pourya Shahpoury, Daniel Štěpánek, Jakub Vinkler, Marco Wietzoreck

YOUNG POSTERS

PY-EnvMonit-01

Use of ceramic passive samplers as an alternative for monitoring contaminants of emerging concern in groundwater
Giacomo Moro, Sergio Santana Viera, Sandra Pérez Solsona, Silvia Lacorte Bruguera

PY-EnvMonit-02

New magnetic sorbent for trace metal analysis in wastewater samples
Sergio J. Abellán-Martín, David Villalgordo-Hernández, Miguel Ángel Aguirre, Enrique V. Ramos-Fernández, Javier Narciso, Lorena Vidal, Antonio Canals

PY-EnvMonit-03

Standardization of microwave-assisted extraction procedures for characterizing metallic nanoparticles in environmental samples by means single particle ICP-MS
Carlos Gómez-Pertusa, Ana García-Juan, M. Carmen García-Poyo, Guillermo Grindlay, Adela Yañez, Luis Gras

PY-EnvMonit-04

Biomonitoring of metals in the urine of children from the Valencian Region (Spain): Levels, predictors of exposure, and risk assessment
Carmen Sáez, Alfredo Sánchez, Yolanda Molina, Trinidad Suelves, Sabrina Llop, Raquel Soler-Blasco, Pablo Dualde, Miguel Ángel Aguirre, Antonio Canals and Clara Coscollà

PY-EnvMonit-05	**The ageing process of peloids from Koviljača Spa (Serbia)** Emilija Vukićević, Aleksandra Šajnović, Nikola Burazer, Gorica Veselinović, Tijana Mutić, Jovana Roganović, Zeki Karagülle, Aleksandar Jokić, Gordana Gajica
PY-EnvMonit-06	**Rapid analyis of chromium species by µLC-ICP-MS** Jelle Verdonck, Katrien Poels, Jeroen Vanoirbeek, Radu Corneliu Duca, Lode Godderis, Erik Smolders
PY-EnvMonit-07	**Electroanalytical sensing of nitrates in cyanobacteria growth media at electrified liquid-liquid interface** Karolina Marciniak, Muthaiah Annalakshmi, Thangaraj S. T. Balamurugan, Karolina Czarny-Krzymińska, Lukasz Poltorak
PY-EnvMonit-08	**Occurrence and potential sources of Polycyclic Aromatic Hydrocarbons (PAHs) in Red river sediments, from Hanoi to the rivermouth (Vietnam)** Khanh Toan Vu, Stéphanie Lebarillier, Thi Quynh Mai Duong, Marc Tedetti, Van Hoi Bui, Vincent Fauvelle, Laure Malleret
PY-EnvMonit-09	***In-vivo* bioavailability of bisphenol A associated to microplastics. Are plastic particles “bioavailability vectors”?** Llucia Garcia-Moll, Francisco Antonio Casado-Carmona, Miguel D. Ferrer, Antoni Sureda, Silvia Tejada, Josep Mercader, Manuel Miró
PY-EnvMonit-10	**Smartphone-based fluorescence imaging system for rapid detection of microplastics in urban stormwater** Marianna Zolyomiova, Fiona Regan, Mercedes Vázquez
PY-EnvMonit-11	**Diatom-derived extracellular polymeric substances affect silver nanoparticles fate in freshwater via eco-corona formation** Rocco Gasco, Isabelle A.M. Worms, Arin Kantarciyan, Vera I. Slaveykova
PY-EnvMonit-12	**Contrasting level of contaminants in different urban land uses depending on the identity** Andrea C. Sala-Navarro, Nuria Casado-Coy, Axel Campos-Castro, Camelia Algora, Elena Aguilar-Santana, Josu G. Alday, Cristina Armas, C. Guillermo Bueno, Leonor Calvo, María Dolores Carmona-Yáñez, Giada Centenaro, Svetlana Dashevskaya, Jorge Durán Humia, María R. Felipe-Lucia, María José Fernández-Alonso, Pablo García-Palacios, Sonia Chamizo, Enrique G. de la Riva, Beatriz Jiménez-Prieto, Juan José Jiménez, Mónica Ladrón de Guevara, María Leo, Ana López-Velasco, Carmen Lorenzo, Manuel Esteban Lucas-Borja, Jesús Pérez-López, Pedro Antonio Plaza-Álvarez, Iván Prieto, Alejandro Terrones, Aurora Torres, Manuel Delgado-Baquerizo, Santiago Soliveres, Ana Beltrán-Sanahuja, Carlos Sanz-Lazaro
PY-EnvMonit-13	**Biodegradable vs. fossil-based mulch: Sorption study of azoxystrobin on pristine and aged particles** Urška Šunta, Ines Merkun, Sara Šariri, Kristina Ugrinović, Mojca Bavcon Kralj

ENVIRONMENTAL SAFETY

P-EnvSaf-01	**Reactivity of malodorous volatile organic sulfur compounds toward hydrogen sulfide** Alexey Kamyshny, Irina Zweig
P-EnvSaf-02	**Human biomonitoring of hexavalent chromium: the potential role of epigenetics within chemical risk management in the workplace** Jelle Verdonck, Manosij Ghosh, Katrien Poels, Lode Godderis, Beata Janasik, Wojciech Wasowicz, Paul T. J. Scheepers, Sophie Ndaw, Radia Bousoumah, An Van Nieuwenhuyse, Radu Corneliu Duca, Susana Viegas, Henriqueta Louro, Maria João Silva, Simo P. Porras, Tiina Santonen, HBM4EU Chromates Study Team
P-EnvSaf-03	**Potentially toxic elements and fatty acids in fish – health risk and benefit predictions for consumers** Tijana Milićević, Snježana Herceg Romanić, Bosiljka Mustać, Jasna Đinović-Stojanović, Dubravka Relić, Gordana Jovanović, Aleksandar Popović
P-EnvSaf-04	**Tobacco sticks and nicotine pouches as an alternative to traditional smokeless tobacco products – comparison of their elemental composition** Aleksandra Pawlaczyk, Paulina Kozieł, Małgorzata Iwona Szynkowska-Jóźwik

YOUNG POSTERS

PY-EnvSaf-01	**6PPD, 6PPD-quinone and other hazardous compounds in tire rubber particles from recreational surfaces** Andres Duque-Villaverde, Daniel Armada, Thierry Dagnac, Maria Llompart
PY-EnvSaf-02	**Evaluation of dermal exposure to antiozonants and other tire rubber compounds present in recycled tire crumb rubber** Andres Duque-Villaverde, Sergio Sóñora, Ana Castiñeira-Landeira, Thierry Dagnac, Maria Llompart
PY-EnvSaf-03	**Bioaccumulation and transformation of plastic additives in hydroponically grown plants: Implications for safe water reuse** Maria Pau Garcia-Moll, Henrry Beral, Lucas Alonso, Lucia H.M.L.M. Santos, Gianlugi Buttiglieri, Sara Rodriguez-Mozaz
PY-EnvSaf-04	**Fibrous microplastic influence on locomotory dynamics and entanglement in *Thamnocephalus platyurus* and *Brachionus calyciflorus*** Matea Marelja, Cuizhu Ma, Huahong Shi, Vera I. Slaveykova
PY-EnvSaf-05	**Understanding the composition of the plastic-associated microbial community in Lake Geneva under different seasonal and spatial conditions and evaluating the biodegradation potential** Laureen Mori-Bazzano, Nhung Nguyen, Vera Slaveykova, Bastiaan Ibelings

POSTER SESSION 2: Thursday 28th, 17:10-18:00

ENVIRONMENTAL TECHNOLOGIES

P-EnvTech-01	**Sorption of pharmaceuticals using layered double hydroxides: considering environmentally relevant conditions** Amy-Louise Johnston, Edward Lester, Orla Williams, Rachel L. Gomes
P-EnvTech-02	**Development of hybrid matrices with photothermal and catalytic functionalities for environmental applications** Mª José Martínez-Tomé, Ahmed Balah Tahiri, Raúl Martínez-Baquero, Felipe Hornos, Javier Gómez, C. Reyes Mateo, Rocío Esquembre
P-EnvTech-03	**Adsorption of aqueous Hg(II) using activated carbons developed from agroforestry biomass: equilibrium and kinetics studies** Amaya Arencibia, Nerea Izquierdo, Gema Gómez-Pozuelo, María-José López-Muñoz
P-EnvTech-04	**Adsorption of carbamate pesticide desmedipham from aqueous solution using reactivated active carbon spheres** Anđelka Tomašević, Dušan Mijin, Denis Dinić, Branislav Stojković, Zlate Veličković, Predrag Stojisavljević, Stevan Stupar
P-EnvTech-05	**MgAl-layered double hydroxide particles for adsorptive removal of Acid Green 25 from aqueous solutions** Anđelka Tomašević, Muna Abdualatif Abduarahman, Marija M. Vuksanović, Nataša Knežević, Milena Milošević, Zlate Veličković[f], Aleksandar Marinković
P-EnvTech-06	**Photocatalytic activation of hypochlorite with graphitic carbon nitride under by simulated sunlight irradiation** André Torres-Pinto, Inmaculada Velo-Gala, C.G. Silva, J.L. Faria, Adrián M.T. Silva
P-EnvTech-07	**TEVA@pipette-tip for on-site SPME of uranium employing a portable smartphone-based colorimetric platform for detection** Andreu Figuerola, Edwin Palacio, Laura Ferrer
P-EnvTech-08	**Phytoremediation of PFAS compounds using wheat seeds treated with alternating electric fields** Branimir Jovančićević, Itana Nuša Bubanja, Marija Lješević, Branka Lončarević, Kristina Joksimović, Kristina Kasalica, Nikoleta Lugonja, Dragomir Stanisavljev, Vladimir Beškoski
P-EnvTech-09	**Boosting reef restoration: Optimization of coral growth with electrochemical technologies** Francisco Montilla, Laura Medina
P-EnvTech-10	**Evaluation of the solar photocatalytic performance of graphitic carbon nitride (g-C_3N_4) on the removal of the insecticide acetamiprid in water** Jorge Plaza Morales, Amaya Arencibia, Paola Calza, Claudio Medana, Federica Dal Bello, María José López-Muñoz
P-EnvTech-11	**Biosorption of amoxicillin and diclofenac from wastewater on modified biochar from buckwheat hulls** Marija Stjepanović, Natalija Velić, Ivan Zdjelarević, Julija Šupljika, Marek Wróbel, Marcin Jewiarz Nikola Maravić, Zita Šereš
P-EnvTech-12	**The influence of pressure changes on the contents and composition of torrefaction liquid products from microalgal biomass** Aleksandra Šajnović, Nikola Burazer, Gorica Veselinović, Urška Šunta

P-EnvTech-13	**Fluorescent nanocomposite eutectogels: a new class of materials for potential environmental sensing applications** Carmen Reyes Mateo, Yolanda Alacid, Raúl Martínez, Francisco Montilla, Rocío Esquembre, María José Martínez-Tomé
P-EnvTech-14	**Synthesis, characterization, and photocatalytic activity of spinel oxide materials** Alaâeddine Elhalil, Wafaa Boumya, Aicha Machrouhi, Rachid Elmoubarki, Noureddine Barka

YOUNG POSTERS

PY-EnvTech-01	**Preliminary study of waste *Paeonia tenuifolia* L. usage for lead ions removal from wastewater** Aleksandar Jovanović, Jelena Dimitrijević, Natalija Čutović Mladen Bugarčić, Tatjana Marković, Jelena Petrović
PY-EnvTech-02	**Remediation of water polluted by potentially toxic elements using biochar from corn and tomato** Emilija Vukićević, Jelena Isailović, Dajana Janjušević, Gordana Gajica, Vesna Antić, Jan Schwarzbauer, Branimir Jovančićević
PY-EnvTech-03	**A new approach for temporal monitoring of reactive oxygen species in advanced oxidation processes** Hugo Clermont, Yongrong Zou, Gilles Mailhot, Mohamad Sleiman
PY-EnvTech-04	**Removal of venlafaxine and diclofenac from drinking water using a *Spirulina*-based carbon bio-sorbent and a commercial adsorbent** Leonor R. Barroca, Ana L.R. Cabral, Marta F. Pedrosa Ana Rita Lado Ribeiro, Adrián M.T. Silva
PY-EnvTech-05	**Functionalized porous sponge of chitosan/alginate with hydrophobic eutectic solvent for paraben extraction in water** J. Mabel Luna-Díaz, Laura Ferrer, Luz O. Leal-Quezada, Edwin Palacio
PY-EnvTech-06	**Treatment of industrial wastewater with a high content of nitrogen compounds in the simultaneous nitrification and denitrification system** Milica Mišić, Mladen Bugarčić, Aleksandar Jovanović, Vladimir Pavićević, Dragan Povrenović
PY-EnvTech-07	**Electrochemical recovery of chromium from tannery industrial wastewater** Paula Pérez, Raúl Berenguer, Emilia Morallón
PY-EnvTech-08	**Effective PFOA electrochemical removal from water using a Ti/SnO$_2$–Sb/PbO$_2$ electrode** Slađana Savić, Dalibor Stanković, Vladimir Beškoski
PY-EnvTech-09	**Hypochlorite activation by spinel ferrites for sulfonamide degradation: Mechanistic insights for potential application in wastewater treatment** Sridhar Gowrisankaran, Armando Zarrelli, Marcello Brigante, Olivier Monfort
PY-EnvTech-10	**Enhanced copper selectivity in multi-element solutions using thiourea formaldehyde-functionalized graphene oxide** Nicole Ferreira, Thainara Viana, Gil Gonçalves, Cláudia Nunes, Bruno Henriques, Eduarda Pereira
PY-EnvTech-11	**Novel photocatalyst for advanced photocatalytical degradation of methyl orange** Aleksandar Jovanović, Mladen Bugarčić, Milica Mišić, Nataša Knežević, Nikola Vuković, Miroslav Sokić, Vladimir Pavićević
PY-EnvTech-12	**Optimization of aqueous phenols sorption in by biomass of African breadfruit** Adaora A. Oguejiofor, Ikechukwu Noel Emmanuel Onwurah, Bennett Chuma Nwanguma, Chukwudi O. Onwosi, Umar Ibrahim Gaya

GREEN CHEMISTRY AND GREEN TECHNOLOGIES

P-GreenChem-01	**Application of ICP-MS for assessing bioaccessibility of metals from food supplements** Lidia Kaynarova, Kristina Guberkova, Deyana Georgieva, Violeta Stefanova
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P-GreenChem-08	**CO_2 conversion: unraveling the effect of hydrophobicity, porosity, and functionalization of nanoporous activated carbon based electrodes** Sebastián Torres, Alicia Gomis-Berenguer, José Solla-Gullón, Conchi Ania, Jesús Iniesta
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PY-GreenChem-05	**Exploring bimetallic Au/Cu nanoparticles as immunosensing platforms** Marian Adeyemi, Andrés Felipe Quintero-Jaime, Ángel Berenguer-Murcia, Diego Cazorla-Amorós, Emilia Morallón
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PY-GreenChem-10	**Functionalized cellulose from deproteinized soybean hulls as an environmental decontamination and disinfection tool** Monica Rigoletto, Amaya Arencibia, María José López Muñoz, María Rapp, Claudia Vineis, Maria Luisa Testa, Maria Laura Tummino, Enzo Laurenti

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P-SustDev-06	**Physicochemical characterization of insulating plastics: a step towards a circular approach to cable recycling** Mališa Antić, Stanislava Gorjanović, Snežana Zlatanović, Darko Micić, Kilino Stojkov, Vesna Antić
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PY-SustDev-02	**Elemental analysis of environmental samples by means microwave-sustained inductively coupled atmospheric-pressure plasma optical emission spectrometry** Jorge Pérez, Paula Gras, Raquel Serrano, Guillermo Grindlay, Luis Gras, Juan Mora
PY-SustDev-03	**HOW to Renew, WHAT to Transform, WHOM to Help – KAJ KO BI** Špela Mihevc, Urška Šunta, Tjaša Bavcon, Mojca Bavcon Kralj
PY-SustDev-04	**Assessment of a deep eutectic solvent for liquid-liquid microextraction of six pharmaceuticals form wastewater** César Castro-García, Luz O. Leal-Quezada, Edwin Palacio, Claudia Domini, Laura Ferrer

ABSTRACTS

PL-01

Climate change and air pollution: two silent killers

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Introduction

The scientific literature widely reports the historical evidence showing unprecedented shifts in global climate over the last two millennia, with recent decades marking the intense period of anthropogenic climate impact [1]. These shifts do not only affect climatic variables, but also atmospheric pollution through modifications in temperature (enhanced photochemistry) and precipitation (removal of aerosols in the atmosphere). These changes also lead to an escalation of wildfires and natural emissions, and therefore exacerbating global health risks and environmental degradation [2].

In this sense, the increase of extreme temperature events under a changing climate can have a substantial impact on public health. These events can lead to fatalities, particularly in vulnerable population groups, although individuals with sufficient exposure are also at risk. Extremely high temperatures are associated with increased mortality, especially during heatwaves, where deaths are primarily attributed to cardiovascular, cerebrovascular, and respiratory causes [3]. Common heat-related syndromes also include heat exhaustion and heatstroke [4].

In addition, atmospheric pollution is a major health risk, contributing to an estimated 6 to 13 million premature deaths annually, with more than 90% of the global population living in areas exceeding the air quality guidelines set by the World Health Organization. Much of the evidence regarding the health effects of air pollution has focused on suspended particulate matter, particularly PM2.5, consisting of particles suspended in the air with a diameter equal to or less than 2.5 micrometers. Multiple epidemiological studies have demonstrated robust associations between long-term exposure to PM2.5 and premature mortality across various health outcomes, including cardiovascular diseases, cerebrovascular events, respiratory conditions, and lung cancer, among other pathologies [5].

The scientific evidence indicates that climate change, propelled by human activities, presents an unparalleled global health challenge. The convergence of climate change and pollution in so-called *compound events* increases the frequency of extreme impacts and health crises, demanding targeted mitigation strategies. This evidence highlights the urgent need for policy frameworks aimed at reducing greenhouse emissions and improving air quality to safeguard human health.

Acknowledgements

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PL-02

Cigarette waste leachates: An overlooked environmental issue

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Text

Cigarette butts are the most commonly littered items in urban areas worldwide, accounting for 22-46% of visible litter [1]. Once disposed onto urban areas, they move through the storm drains to streams, into the ocean, and back onto the beaches. This makes cigarette butts the single most collected item in coastal environments each year, and the second most found item on beaches in the European Union [2]. Environmental awareness on the disposal of tobacco products mainly focuses on the inability of discarded filters to biodegrade. There is markedly less awareness on the potential of TPs to act as point sources and leach toxicants [3,4]. To this end, leachates from discarded cigarettes have been shown to be acutely toxic for different species such as marine bacteria (Vibrio fischeri), fish, snails and fish and frog embryos [3].

The present contribution presents the inorganic and organic chemical components of environmental importance that are leached from used and unused tobacco products. Conventional cigarettes and the new generation Heat-not-Burn product are considered. The contribution of the different parts of tobacco products to the inorganic and organic content of leachates was assessed and compared to the total concentration of each chemical constituent initially present in the tobacco product. HiSorb high capacity sorptive extraction uses PDMS-based probes for the extraction of PAHs directly from the complex leachates Cigarette leachates consist of highly complex mixtures of compounds across a wide concentration range, and such compounds typically elute as an unresolved complex mixture when subjected to one-dimensional gas chromatography (GC). Comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry (GC×GC-TOFMS) with high-capacity sorptive extraction was therefore used for the exploratory profiling of leachates from used and unused cigarettes. Comparison of the results to those obtained from unused tobacco products allowed identifying the toxic compounds formed during the burning or heating process (depending on the product). All in all, the false perception that discarded tobacco products are the end point of a life cycle, points that there is still a way to go in addressing responsible disposal and post-consumer waste cleanup, so as to minimize the environmental hazards of discarded tobacco products.

Acknowledgements

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KN-01

Birds as biomonitors of environmental pollution

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Introduction

Biomonitoring is the measurement of chemical compounds and/or their metabolites accumulated in biological systems, and is used around the world as reflect the quality of the environment and can infer potential adverse effects to wildlife. Biomonitoring strategies are gaining importance within the context of the Birds and Habitats Directives (2009/147/EC and 92/43/EEC), the Zero Pollution Action Plan and the new European Biodiversity Strategy aimed at reversing biodiversity loss in the EU. In this study, we propose the use of gull eggs (*Larus michahellis*) and the protected species (*Larus audouinii*) as biomonitors of legacy and emerging contaminants (Zapata et al., 2018; Colomer-Vidal et al., 2022). Gulls are long-lived, have a wide distribution and are tolerant to environmental pollution, thus reflecting contaminant variability over a protracted period. Our biomonitoring strategy includes the analysis of multiple contaminants such as polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), perfluoroalkyl substances (PFASs), polybrominated diphenyl ethers (PBDEs), polycyclic aromatic hydrocarbons (PAHs), dechlorane plus, short-chain chlorinated paraffins and phthalates. Several solid-liquid extraction protocols have been optimized and validated to determine the different chemical families. Analysis is performed with gas and liquid chromatography coupled to tandem mass spectrometry (LC or GC-MS/MS) or coupled to high-resolution mass spectrometry with an Orbitrap or time of flight mass analyzers for the non-targeted approach to extend the number of other potential contaminants present in the samples. Our results reveal specific geographical contamination patterns according to the anthropogenic pressures in each sampled colony and time variations related to the use and prohibitions of several commercial formulations. Also, the use of gull eggs as biomonitors permit to evaluate the impact of environmental pollutants in other species sharing habitat and with similar diet, as observed for flamingos (*Phoenicopterus roseus*) or shearwaters (*Calonectris diomedea*). Overall, we propose the use of gull eggs as environmental biomonitors to identify the pollution status of areas of high ecological interest and to contribute to the implementation of management and conservation actions against chemical pollution.

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KN-02

Polycyclic aromatic compounds – atmospheric fate and environmental exposure

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Introduction

Many polycyclic aromatic hydrocarbons (PAHs) and their nitrated (NPAHs), oxygenated (OPAHs) and halogenated (XPAHs) derivatives are toxic and ecotoxic [1-5]. NPAHs and OPAHs are co-emitted with PAHs from fossil fuel and biomass combustion processes, or are formed in photochemical and microbiological reactions of PAHs in air and soil [3, 6-7]. Despite laboratory and field studies of these pollutants' sources, photochemistry and occurrence in air, little is known about atmospheric lifetimes and environmental fate on large spatial scales. As semivolatiles resisting biodegradation in soils and surface waters, their long-range transport potential is enhanced by multihopping (grasshopper effect) [6, 8].

Features of large-scale distributions and atmospheric cycling of selected PAHs and NPAHs are highlighted based on recent advances in modelling of sources, transports and photochemistry [9-11]. Some PAHs and OPAHs are found to be globally distributed, but overall little is known about large-scale distributions and exposure of remote environments, including the open oceans [11-12]. The multihopping potential was explored in soils of source and receptor sites [13], and in surface seawater. Because of neglected re-emissions (secondary sources), PAH emission inventories may be underestimated, in particular in receptor areas.

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KN-03

Are we aware of the role of enantioselectivity in the environment?

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Introduction

Many pharmaceuticals are chiral, *i.e.*, asymmetric three-dimensional molecules with stereoisomers that can display a different behaviour in chiral medium, as occurs in the interaction with natural macromolecules (*e.g.*, enzymes, receptors, other binding-molecules). Therefore, enantiomers may have different pharmacokinetic and/or pharmacodynamic properties due to the different attachment to the binding sites and dissociation from them [1]. In the case of pharmaceuticals, they may be administered as enantiopure or enantiomeric mixtures. In fact, the potency, mode of action, and toxicity can differ for a pair of enantiomers. As example, the antibiotic ofloxacin is sold either as racemate or *S*-(-)-ofloxacin (levofloxacin), levofloxacin having a lower minimal inhibitory concentration and less incidence of adverse effects. Consequently, enantioselectivity can also occur in all biological processes occurring in the environment [2]. Therefore, different responses in terms of ecotoxicity are also expected [3]. This communication aims to highlight that although chirality is rarely considered in environmental studies, the knowledge on stereoselectivity in the environmental fate, distribution, (bio)transformation, (bio)degradation, ecotoxicity, and bioaccumulation is essential to provide a more realistic environmental risk assessment of chiral pharmaceuticals. Examples of enantioselective environmental studies will be presented.

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KN-04

Suspect and non-target screening of persistent organic pollutants in environmental samples by two-dimensional gas chromatography−time-of-flight mass spectrometry

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Introduction

The increasing awareness of our environment as a source of human exposure to a large number of known and unknown chemicals has promoted a growing interest in holistic approaches allowing a more complete evaluation of the contaminants present in the matrices investigated. This appreciation has increased interest in performing suspect screening (SSA) and non-target screening (NTS) analyses complementary to the target monitoring of well-know and regulated micropollutants over the past decade. These two types of analyses differ in the sample preparation procedures required and the techniques used for final instrumental analysis of the generated extracts. Regarding this last analytical step, compared to target procedures, SSA and NTS analyses require an enhancement on either the separation capability or the detection power of the technique used for final analyte determination. In practice, this meant that single-column instrumental techniques have usually relied on the use of high-resolution mass spectrometry (HRMS), i.e. LC-HRMS for polar analytes, and GC-HRMS for medium and non-polar analytes. However, the enhanced separation power provided by comprehensive two-dimensional gas chromatography, combined with the identification capabilities derived from its hyphenation with time-of-flight mass spectrometry (GC×GC–ToF MS) has also been proved to be advantageous in this type of determinations.

In this communication, the feasibility of GC×GC–ToF MS for SSA and NTA will be illustrated through selected application studies addressing the characterization of persistent organic pollutants (POPs) and POP-like analytes in complex environmental matrices. The different levels of confidence achieved for the proposed identifications will also be discussed.

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KN-05

Organic UV Filters as indicators of antropogenic micropollution in insular ecosystems

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Introduction

Organic Ultraviolet Filters (UVFs) are used to protect the skin against the harmful UV radiation effects such as sunburns, photo-aging and skin cancer [1]. The concern about the overexposure related with the tendency to spend more time under the sun, has led the growth of solar protection industry. Organic UV filters are employed in different personal care products (PCPs) such as lotions, cosmetics, shampoo and soaps. Furthermore, these compounds are also added to industrial goods, such as paints, textiles, plastics, disinfection products and detergents. However, some UV filters present unwanted dermatological effects such us dermatitis or allergies. Due to their extensive use, hundreds of tons of organic UV filters are released to the environment annually considering them as a new kind of environmental pollutants which may produce adverse effects on ecosystems.

In this lecture, we present several cases studies about the presence of Organic Ultraviolet Filters in different marine ecosystems from an insular region, specifically, the Canary Islands. The Canary Islands is an archipelago of Atlantic islands made up of eight islands, with a total population of approximately 2.223.951 inhabitants, and whose main source of economy is tourism, having received more than 15 million tourists last year. Then, the sea surrounding this archipelago suffers great anthropogenic pressure due to domestic and touristic activities. Thus, in this presentation we will focus on monitoring and impact studies of UVFs in marine coastal waters, marine organisms and microplastics from different locations of this Atlantic archipelago [2], [3] [4].

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KN-06

Biochemical strategies for valorisation of agrifood waste and side streams for a circular primary sector

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Introduction

Providing the world's population with food in a way that is both sustainable and contributes to human health and well-being is a major global challenge. Today's food sector has a very high environmental footprint, and it is pressing our planetary boundaries with harmful effects on, among other things, climate and biodiversity. Indeed, food production alone contributes to one quarter of the world's total greenhouse emissions.[1] At the same time, 38% of food produced is globally lost and wasted throughout the entire value chain. Agricultural by-products and food waste therefore constitute a huge environmental burden accounting for 10% of total greenhouse gas emissions, and lead to huge economic losses costing $2.6 trillion annually.[2] This highlights the urgency to transition into a sustainable and circular food system, making use of the waste and side streams generated in all steps of the food system, from farm to fork.

Food waste and loss (FLW) streams frequently contain edible or usable materials that can be reintegrated into the food supply chain through safe processing, presenting an opportunity to increase food availability without additional strain on agricultural resources. Different technological approaches can be envisioned to process such FLW streams, based on biological, chemical and physical processes, and transform them into a wide array of valuable products, such as different inputs needed for food production (ie. bioenergy, fertilisers, bioplastics) together with feed and food for animal and human consumption. However, when discussing different approaches, the hierarchy for food waste management needs to be considered, ensuring that the most benefit is made from the rich composition and volumes of the existing FLWs.

In this presentation we will discuss the challenges and opportunities for the valorisation of agrifood FLW from different sources. In particular we will focus on different chemo-enzymatic routes fusing green extraction processes and enzyme technology for the transformation of solid and recalcitrant side streams from plant production (ie cereals and fruits) into valuable food ingredients with potential benefits for human health. We will discuss the implementation of subcritical water extraction for the isolation of valuable dietary fibres and phenolic compounds from cereal and fruit side streams[3, 4]. Moreover, enzyme technology can be used for the generation of valuable prebiotic oligosaccharides and for the engineering of food ingredients (ie texturisers and emulsifiers) with both functional and nutritional benefits.[5, 6] The health benefits of introducing dietary fibre food ingredients in our diets will also be discussed. All in all, our biochemical strategies to upcycle FLW into healthy and functional food ingredients contribute both to improve the circularity of the food system and address current nutritional gaps in the consumption of dietary fibres in our diets.

Acknowledgements

The authors acknowledge the Swedish Research Council FORMAS (2020-01575) and Novo Nordisk Foundation (NNF21OC0071410) for their financial support.

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KN-07

Physiologically-based extraction assays of plasticizers from microplastics: Is the ˈTrojan-horseˈ effect hype or reality?

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Introduction

There is a plethora of studies investigating the impact of microplastics (MP) and nanoplastics (NP) in the food web and marine and terrestrial biota for potential metabolic disorders, yet the role of plastic-laden compounds is sometimes neglected because of the lack of proper characterization of the samples under study [1]. In those works contemplating the release of plastic-related compounds after MP/NP ingestion, overly simplistic gut fluids of marine biota, in terms of number of gut compartments, and chemical composition (sometimes only pH adjustment or addition of surfactants), has been often resorted to risk assessment explorations [2].

To tackle those issues, this invited lecture gears towards the implementation of physiologically relevant extraction tests for reliable assessment of the oral bioaccessibility of plastic monomers and additives [3-5], as demonstrated with the analysis of certified reference materials of medium-density polyethylene (PE) and polyvinylchloride (PVC) MP containing phthalate congeners and bisphenol A. To elucidate whether the Trojan-horse effect of MP is hype or reality, we have developed a multi-compartment oral bioaccessibility test to mimic the gastrointestinal tract (GIT) of marine vertebrate and compared the plasticizers intake via MP or dissolved in seawater using cumulative probability curves at the 10th, 50th and 90th percentiles [6]. Extension to the human gastric and gastrointestinal compartments under fasted and fed-conditions is also demonstrated [7]. Our results, supported by recent literature, evince that the vector-like effect of MP for incurred additives and plastic monomers is usually negligible.

However, it should be noted that the standard physiologically-based tests are usually performed under static batch conditions, whereby the dynamic nature of the GIT of biota is not properly simulated. Therefore, this lecture will illustrate how flow-through oral bioaccessibility tests can be fully automated by resorting to advanced flow approaches integrating clean-up of the body fluids and preconcentration of the bioaccessible organic targets from MP prior to liquid chromatography [8]. Similar flow systems can be assembled to explore the leachability of plastic additives in marine settings without potential sink constraints of the standard leaching methods [9]. Besides the analysis of primary MPs, this lecture will also offer experimental data of the oral bioaccessibility of parent additives and thermal/phototolytic degradation by-products of aged MP after weathering the same reference PE/PVC MPs in a climate chamber for about 2 months.

Acknowledgements

The authors acknowledge the financial support provided by the Spanish Ministry of Science, Innovation and Universities (MICIU), the Spanish State Research Agency (AEI/10.13039/501100011033) and the European Union (NextGenerationEU/PRTR) through the projects PID2020-117686RB-C32 (MICIU/AEI), PID2020-117686RB-C33 (MICIU/AEI), and TED2021-131303B-I00 (MICIU/AEI/NextGenerationEU/PRTR).

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OS-01

Latest trends in PFAS testing and regulations landscape

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Introduction

We all knows that do tell PFAS is really not enough to make people understand what we do speak about, different lengths, different functional groups, different matrices, the most ever confusing regulation make the PFAS issue one of the most problematics

Which are the technologies used to analyze them and when is better to use a certain technology other than another?

Most recent analytical trends for PFAS and directly connected problems that we do need to be aware of This presentation aim at provide a clear and focused overview of the Pfas analytical world

OS-02

Enhancing non-targeted analysis using comprehensive-two-dimensional gas chromatography coupled to a high-resolution mass spectrometry in environmental samples

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Introduction

Modern society produces, markets, and uses an increasing number of chemicals, which can be released into the environment through various pathways. The adoption of Non-Target Screening (NTS) workflows to identify these chemicals in the environment and organisms using high-resolution mass spectrometry has rapidly grown within the research community. The combination of comprehensive two-dimensional gas chromatography with high-resolution time-of-flight mass spectrometry (GCxGC-HR-TOFMS) is a powerful analytical technique for NTS of complex samples. This combination offers enhanced chromatographic separation and high-speed acquisition of accurate mass spectra across the full mass range. The generation of such rich data enables insightful retrospective review for vast numbers of unknown compounds. Additionally, target analysis can be performed simultaneously using the same data set obtained for NTS.

A systematic workflow is presented here for screening both target and non-target contaminants in various high-complexity samples. A combination of non-polar and polar stationary phases was used to enhance separation power of the GCxGC method adopted, resulting in better resolution between matrix and target compounds and, consequently, purer MS spectra for target POPs such as PCB, BDE, and Toxaphenes. Identification and confirmation were achieved through the injection of native standards and the application of dedicated targeted-processing methods. A novel Multi-Mode Source (MMS), capable of EI/CI (both positive and negative), was used to enhance identification confidence by providing library-searchable spectra, accurate mass, and molecular ion information for formula support and/or determinations. For this work, primarily EI and ECNI ionization modes were employed, with ECNI preferred for molecular ion information and formula support in cases where the identity of non-target substances could not be confirmed by EI ionization.

A list of target and non-target molecules is presented, along with information about identification methods (e.g., native standard, retention time, retention index, mass accuracy, etc.). EI high resolution mass spectra will be showed along with ECNI spectra used for confirmation. Formula computation approaches will be highlighted.

The benefits of GCxGC in providing superior separation capabilities and structured chromatograms are highlighted, along with the importance of the novel multi-mode source for HR-TOFMS, which allows for three ionization modes without hardware changes. The combination of ECNI spectra and EI information, such as retention time, retention index, and tentative identification through commercial databases, provided significant information that helped confirm the presence of halogenated POPs in the measured samples.

OS-03

Accurate microplastics characterization on water samples with aluminum-coated filters using QCL IR chemical imaging

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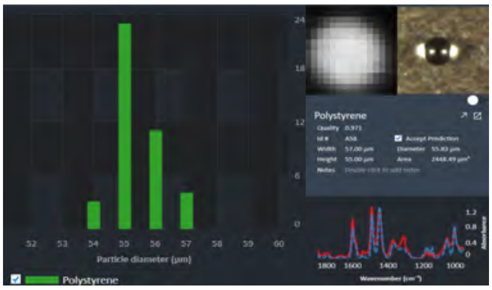
Introduction

Indeed, microplastic pollution has become a significant environmental concern due to its potential impacts on ecosystems and human health. QCL Infrared Chemical Imaging System represent an innovative approach to imaging and spectral analysis, particularly in the context of microplastic identification and other applications that require chemical characterization of materials.

The new directive (EU) 2020/2184 has been developed to ensure the safety of water intended for human consumption. This directive includes a comprehensive methodology to measure microplastics in drinking water with the use of vibrational spectroscopy techniques. QCL IR imaging systems are one of the newest technologies allowing the counting, characterization, classification and identification of microplastics on a faster and more cost-efficient way.

Microplastics water analysis is performed after a filtration step using 100 and 20 microns sieves. The retained particles are usually transferred to low e-slides or gold coated filters for measuring. To minimize the cost associated with gold-coated filters while maintaining easy and efficient sample introduction method, accurate microplastics characterization with IR QCL can be performed on aluminum-coated PET and PC filters. This study outlines the utilization of QCL IR Imaging in achieving accurate microplastics characterization on aluminum-coated filters. Results showing the capabilities of the QCL in terms of particle detection, particle count repeatability, particle size accuracy and identification of common microplastics will be shown.



Polystyrene
Quality 0.971
Id # A58
☑ Accept Prediction
Width 57.00 µm
Diameter 55.83 µm
Height 55.00 µm
Area 2448.49 µm²
Notes

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OS-04

From Known to unknown in Mass Spectrometry: An example with PFAS Challenge in environmental samples

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Introduction

In this presentation, we will address the analytical challenges associated with the determination of per- and polyfluoroalkyl substances (PFAS) across various matrices and scenarios. Given the extensive family of PFAS compounds and their ubiquitous presence, their determination represents one of the most intriguing and demanding analytical challenges in contemporary environmental chemistry.

We will show an optimized workflow for the analysis of a legally mandated list of PFAS compounds in environmental samples. This workflow leverages the advanced capabilities of the new LCMS DART TQ+ Platform, ensuring ultimate sensitivity and robustness.

Additionally, we will explore complementary approaches for PFAS family identification and non-target analysis. Utilizing cutting-edge high-resolution mass spectrometry systems, with or without trapped ion mobility devices timsTOF, we will showcase analytical workflows designed to address this complex analytical puzzle.

O-01

Advances in the electrochemical reduction of CO_2 into formate/formic acid

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Introduction

The electrocatalytic reduction of carbon dioxide (CO_2) to formate ($HCOO^-$) or formic acid (HCOOH) represents a promising alternative for mitigating CO_2 emissions into the atmosphere [1]. Also, interestingly, both $HCOO^-$ and HCOOH can be used as raw materials with numerous and diverse applications in industry. In this work, some of our advances in the application of Bi, Sn, and Sb nanostructured based electrocatalysts for the selective conversion of CO2 into HCOO-/HCOOH will be presented and discussed [2-5]. This presentation will cover from fundamental aspects, including the synthesis, characterization and electrocatalytic properties of these nanostructured materials on conventional H-type electrochemical cells, to practical applications, focused on the development and testing of an electrochemical filter-press reactor working in a continuous operation mode. Also, our recent advances to improve the electrochemical process using alternative anode reactions (electrooxidation of glycerol) instead of the traditional oxygen evolution reaction (OER) [6-8] will be presented and discussed.

Acknowledgements

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O-02

Semi-volatile organic pollutants in the Polar Arctic atmosphere: Long-term passive sampling and GC-HRMS analysis

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Introduction

Studying the chemical composition of the high-latitude atmosphere is key to understanding global trends associated with climate change and economic development in the Arctic. So far, the most environmental monitoring studies in the Arctic were aimed at targeted analyses of a limited range of specific priority compounds. However, the number of emerging pollutants is constantly growing, and the existing knowledge about their chemical composition and transformations is scarce. Due to the low levels of pollutants, remoteness and poor accessibility of the polar region, searching, identifying and quantifying the emerging compounds is an extremely complex task and requires implementing advanced analytical techniques.

In the present study, the combination of the long-term (185 days) passive sampling (Radiello radial diffusion sampler with 250 mg of the Tenax-TA sorbent) and thermal desorption GC-MS with Orbitrap mass analyzer was used to identify organic pollutants in the air of the Alexandra Land island (Franz Josef Land archipelago) located north of the 80th parallel. More than 400 semi-volatile compounds belonging to the different classes (CH, CHO, CHN/CHON and CHOS, CH-Hal/CHO-Hal (Cl, Br, F), and CHO-Si) were detected and their elemental compositions were calculated (Figure 1). Most of them were identified at 1-3 confidence levels. Along with 38 EPA priority pollutants, a large number of new compounds, including oxygenated PAHs and unusual trifluoromethyl-substituted halogenated aromatic compounds, were found.

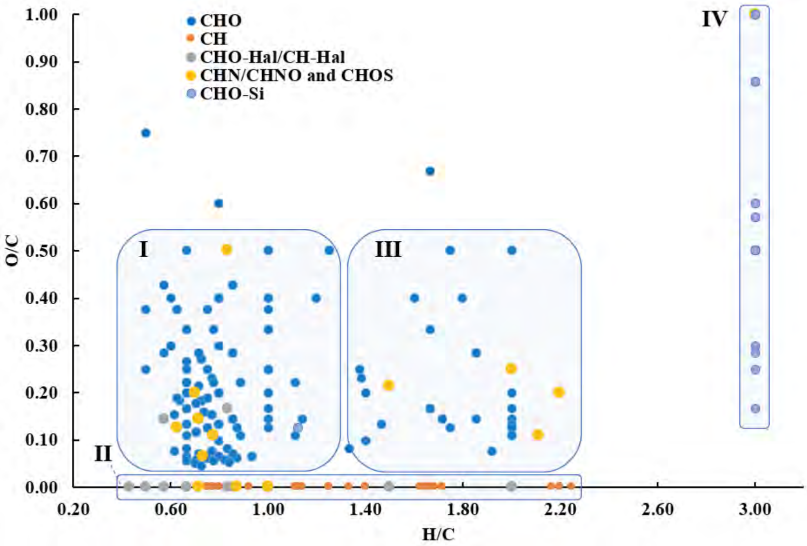

Figure 1 – Van Krevelen diagrams (O/C vs. H/C) of the compounds detected in air samples: Oxygen-rich alicyclic and aromatic structures, including oxy-PAHs (I), Oxygen-free aromatic and aliphatic structures (II) Aliphatic-like structures and aromatics with long aliphatic chains (III) Organosilicon compounds (IV)

Acknowledgements

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O-03

Bioaccumulation, organotropism and toxicological risk of trace elements in *Caretta caretta* (Linnaeus, 1758)

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Introduction

The present study compares the concentration of trace elements (TEs) found in different tissues and eggs of the loggerhead sea turtle, with a view to evaluating the potential toxicological risk for this important bioindicator species [1]. A total of 18 elements were analysed through inductively coupled plasma mass spectrometry (ICP - MS) from nine individuals of *Caretta caretta* that had been found stranded along the northwest coast of Sicily (Italy), as well as from the shells and yolks of six eggs from the island of Linosa (Sicily Strait, Mediterranean Sea). The elements analysed exhibited organotropism, with the highest bioaccumulation levels observed in the liver. The highest concentrations of iron were found in the livers, followed by zinc in the hearts and arsenic in the kidneys. While the levels of most trace elements were comparable to those previously documented, the elevated concentrations of arsenic and cadmium in the kidneys and liver suggest the potential for adverse effects associated with exposure to these non-essential elements. With regard to the eggs, the most prevalent elements in the yolk were zinc, iron, and barium, while iron, boron, and copper were the most abundant in the eggshell. As several of the trace elements identified in *C. caretta* eggs have not been previously analysed, comparisons with other studies in the literature have not been possible.

The findings of this study represent a preliminary investigation that paves the way for further research in this area and emphasise the crucial role of multi-element biomonitoring in assessing potential threats to *C. caretta* adults and eggs, and their implications for the survival of this endangered species. Furthermore, this biomonitoring study enables the evaluation of prevailing TEs pollution levels, thereby supporting the formulation of appropriate environmental policies and regulations.

Acknowledgements

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O-04

Biodegradation of bisphenol A and its analogues by green algae and cyanobacteria

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Introduction

Bisphenol A is one of the highest production volume chemicals used in the production of epoxy resin, polycarbonate plastics and thermal paper. The toxicity and estrogenic activity of this compound has led to restrictions on its use, and many analogues have been produced to replace it in a number of consumer products. Unfortunately, bisphenol analogues are not a safe alternatives. Due to their ubiquity in the environment, increasing attention is being paid to finding an ecological method of removing these pollutants from the aquatic ecosystems [1].

The main task of this research was to investigate the removal efficiency of bisphenol A and its selected analogues, such as bisphenol AF, bisphenol B, bisphenol C, bisphenol E, bisphenol F and bisphenol Z by green algae *Chlorella fusca* (BA-18), *Kirchneriella obesa* (BA-51) and cyanobacteria *Anabaena aphanizomenoides* (LEGE 00250), *Cylindrospermopsis raciborskii* (LEGE 97047). Green algae cells were purchased from the Culture Collection of Baltic Algae and cyanobacteria cells were acquired from the Blue Biotechnology and Ecotoxicology Culture Collection. Exponentially growing strains were exposed to 0.5 mg/l mixture of bisphenol A and its selected analogues for 14 days. The concentrations of the tested compounds in the control sample (the amount of abiotic removal) and in the test sample (the amount of biotic removal: residual amount in the medium, amount adsorbed on cells and accumulated in cells) were determined using a high-performance liquid chromatography system equipped with a diode array detector or a fluorescence detector (Agilent Technologies, USA) and InfinitlLab Poroshell 120 EC-18 (4.6 ×150 mm, 2.7 μm) column.

The results of this study suggest that green algae, compared to cyanobacteria, show a high ability to remove bisphenol A and its selected analogues from the aquatic environment and can be successfully used to remove these contaminants from the aquatic ecosystems.

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O-05

Ceramic passive samplers for the analysis of organic contaminants in water

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Introduction

Passive sampling is one of the most economically and technically feasible approaches to water sampling for the control of organic contamination. Due to the property of passive samplers to accumulate contaminants over the whole sampling period, this technique can provide representative data in time (time weighted averages) without increasing the number of required analyses and costs per sample (Figure 1).

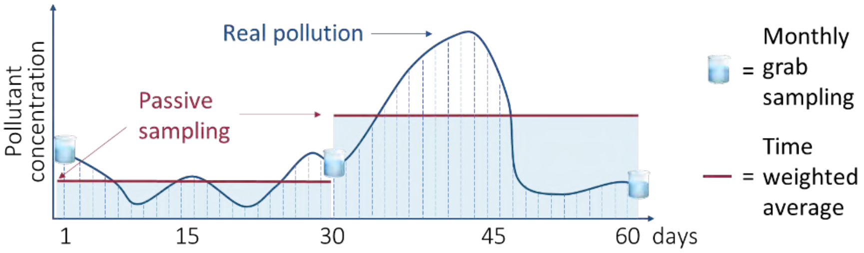

Figure 1. The comparison between monthly grab sampling affording punctual contaminant concentrations (beakers), monthly passive sampling producing time averaged concentrations over a month (red line), and real variations of contaminant concentration in time (blue line).

This communication presents the development of ceramic passive samplers (CPS) for monitoring of organic contaminants in water. The simple design of CPS is represented by a porous ceramic cylinder with two caps and an absorbent placed in the inner volume (Figure 2a). Contaminants diffuse from the water to the inner part of the cylinder, where they are retained by a sorbent. One of the advantages of the CPS is that the porosity and dimensions of the ceramic membrane can be customized (Figure 2b,c), allowing a high adaptability to various requirements of sampling periods and water types. Deployment of CPS in waters allows the monitoring of organic contaminants in a time integrated manner, allowing the assessment of the pollution status.

Figure 2. a) The design and components of CPS, b) three CPS models with different dimensions, c) diffusion of methylene blue through the membrane over time for the three different CPS geometries.

Acknowledgements

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O-06

Combining waste PET-MIL-101(Fe) and cellulose acetate polymeric membrane for the preconcentration and extraction of neonicotinoid insecticides in water samples

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Introduction

Neonicotinoids are the first new class of insecticides introduced more than 50 years ago [1]. Due to their wide use worldwide to fight unwanted insects from attacking crops, these compounds are currently the most used insecticides in the world [2]. However, due to their wide use in agricultural activities and their hydrophilic characteristics, they have been detected in portable water [3] wastewater [4], groundwater [5] and surface water [6]. Although these neonicotinoid insecticide residues have been detected at low environmental concentrations, their constant release to various sources could lead to emerging concerns regarding long-term exposure to human health and other living organisms [7,8]. Therefore, there is an urgent need for intensive environmental water monitoring campaigns, especially neonicotinoid residues, because it has been reported that long-term exposure to these insecticides is associated with adverse human health effects such as pulmonary impairment for adults and weakened intellectual development for children. A MIL-101(Fe) based polymer membrane was successfully synthesized and applied for the preconcentration and quantification of neonicotinoid insecticides (NIs) in water samples using direct immersion-thin film microextraction method (DI-TFME). The selected NIs were detected and quantified using high performance liquid chromatography coupled with diode array detector (HPLC-DAD). The parameters affecting the extraction efficiency of the method and preconcentration processes, such as pH, sonication time, elution time, and eluent volume, were optimized using central composite design. At optimum experimental conditions, limit of detection (LOD), limit of quantification (LOQ) and linearity obtained were 0.013-0.016 µg/L, 0.043-0.053 µg/L and 0.04-500 µg/L, respectively. The intraday (repeatability) and interday (reproducibility) precisions expressed as relative standard deviations (%RSD) were 1.2-2.7% and 3.3-3.9%, respectively. The enrichment factors were 73, 74, 75 and 88 for clothianidin, imidacloprid, thiacloprid and thiamethoxam, respectively. The method was finally employed for determination of selected neonicotinoid insecticides in real water samples.

Acknowledgements

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O-07

Application of passive samplers for the evaluation of trace metals in the Llobregat River basin, Spain

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Introduction

The prolonged drought in the Catalonia region makes it crucial to assess both the quality and quantity of water that supplies the population. Les Fonts del Llobregat, located in the upper part of the Llobregat River basin and serving over 3 million people, are crucial for this monitoring [1]. However, water quality monitoring faces significant challenges due to the large number of samples required, their transportation and analysis, and the associated costs. The use of passive samplers emerges as an innovative solution, especially for hard-to-reach areas. These samplers integrate punctual variations over time, becoming a valuable tool for qualitative and quantitative water quality monitoring. They offer a more comprehensive and accurate perspective while minimizing the challenges of traditional monitoring methods.

The objective of this study is to implement passive samplers, specifically Diffusive Gradient in Thin-Films devices (DGTs), in the upper area of the Llobregat River basin) [2]. A total of 30 sampling points were established throughout the upper area of the Llobregat River basin, including rainwater, spring water, surface water, and groundwater samples. Water grab samples were collected at sampling points for subsequent analysis of major and trace metals by ICP-OES and ICP-MS, respectively. Additionally, DGT devices were deployed in the piezometers and collected after 40 days. The DGTs used consist of a binding layer based on a chelex-100 resin, which can measure up to 30 metals, including Cd, Co, Cu, Fe, Mn, Ni, Pb, and Zn among others [3, 4], and a gel of polyacrylamide as the diffusion layer placed on top (see Figure 1). Moreover, during a second sampling campaign, Polymer Inclusion Membranes (PIMs), were included as a passive device. These PIMs are composed of the TOMATS extractant and CTA as a carrier [5].

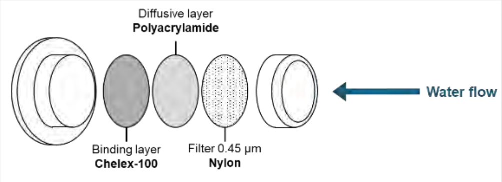

*Figure SEQ Figure * ARABIC 1 DGT composition*

This presentation will provide a characterization of the study area focused on mobility and bioavailability of metals through the analysis of the collected water samples. This will allow us to interpret the water cycle of the upper Llobregat River and to manage the water quality in the sampling area. Furthermore, the application of passive devices will complement the study, providing additional information regarding the bioavailability of the studied compounds.

Acknowledgements

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O-08

Impact of agricultural emissions on rural and urban air quality (IMAGE)

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Introduction

Air quality is of paramount importance to human health. This is recognised by numerous agencies, most notably the World Health Organisation. Adverse health impacts are associated with air pollutants, many of which are linked with anthropogenic / agricultural activity. These pollutants include particulate matter (PM), nitrogen oxides and ammonia among others and have been heavily linked with health concerns and in the secondary formation of deleterious compounds and aerosols. PM can be broken down into size factions, with the terms $PM_{2.5}$ and PM_{10} (referring to PM smaller than 2.5 and 10 microns respectively) generally used in monitoring. PM can also be defined by the pathway it enters the air, with primary PM being directly released to the atmosphere and secondary PM being formed in the atmosphere through chemical reactions involving primary emissions. In this regard the contribution of ammonia to the fine particulate matter fraction through secondary aerosol formation is underdeveloped in an Irish context.

Ammonia emissions is one of the key challenges to agricultural expansion in Ireland. By the end of 2018, total cattle numbers were approaching 6.6 million, while the number of pigs was approaching 1.6 million and increasing. The number of poultry stands around 11 million, with the majority (7.6 million) being in the Border region.[1] Ireland is committed to the EU National Emissions Ceilings Directive (2016/2284/EU), which sets emissions reduction targets for five important air pollutants: nitrogen oxides, non-methane volatile organic compounds (NMVOCs), sulphur dioxide, ammonia and $PM_{2.5}$. These pollutants contribute to poor air quality, leading to significant negative impacts on human health and the environment. Ireland is obliged to reduce ammonia emissions by 1% per year compared to 2005 levels in the years until 2029 and 5% annually thereafter. By the same directive, Ireland is obliged to reduce $PM_{2.5}$ by 18% compared to 2005 levels until 2029 and 41% annually thereafter.[2] Ireland exceeded the emissions ceiling for ammonia in 2016 and 2017 and total ammonia emissions are projected to be 9.6 kt above target in 2020. A reduction in ammonia would also lead to reduction in ambient $PM_{2.5}$ levels.

The health concerns associated with PM makes understanding its formation, concentration, composition, and size regime in both urban and rural settings is of the utmost importance and is the main driver underpinning the work presented here. IMAGE will determine the concentrations of both fine PM and ammonia at two different sites within Ireland. This will be undertaken via the combination of highly accurate and precise offline chemical and biological analysis of collected filter samples and real-time PM and bioaerosol concentration determination of the fine and course fraction of PM. This multi/interdisciplinary work, evaluating ambient environment will provide information of both primary emissions of PM and secondary formation from precursors such as ammonia. Determination of primary sources of $PM_{2.5}$ will greatly aid in the deconvolution of the secondary fraction of $PM_{2.5}$. Equally an understanding of the production of bioaerosols in the fine faction is a novel undertaking.

Acknowledgements

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O-09

LC-HRMS response to the mystery of nano/microplastics: A study focused on detection and identification of plastic polymers and their photooxidation products

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Introduction

Improperly managed plastic debris highlights the significant human impact on the environment, prompting a need for sustainable practices. This debris degrades water quality, and our understanding of plastic particles' behavior, particularly nanoplastics, is still limited. Micro/nanoplastics, which arise from the breakdown of larger plastics, are not well addressed in wastewater treatment and pose unique challenges, requiring an urgent boost in research due to their widespread presence and potential environmental impact. In this view, a complete characterization of nanoplastics is necessary to direct research experimenting with safety evaluation. A key question concerning the aforementioned, which is still unanswered, is their reactivity with environmental substances and interaction with other contaminants, possibly leading to the degradation of products and transformation processes. Another unresolved mystery is the possible presence of “ghost plastics”, which are tiny relatively unknown nanoplastics. The major hurdle in understanding these is the lack of proper detection and quantification. Our present work addresses these issues by investigating the detection of nano/microplastics and identifying possible degradation products. We tackle this problem first developing methods to detect several micro/nanoplastic polymers (such as polystyrene-co-acrylonitrile (SAN), polymethacrylonitrile (PMA), polycaprolactone (PCL), polylactic acid (PLA), polypropylene (PP), polystyrene (PS), polystyrene-co-divinylbenzene (PSDVB), etc.) using liquid chromatography high-resolution mass- spectrometry (LC-HRMS). Using LC-HRMS offers several advantages over previously researched Py-GC-MS for analyzing nanoplastics, like low detection limits, analysis of complex mixtures, diverse analytes, and their degradation products. Firstly, the Exploris™ 120 hybrid quadrupole-Orbitrap™ mass spectrometer was used to understand the characteristic *m/z* signals corresponding to the different plastic polymers employing dual ionization mode and scanning ranges of 40-500 *m/z* and 500-1500 *m/z*. We have observed that this procedure was fundamental for acquiring a fingerprint pattern of *m/z* losses occurring inside the MS for a typical micro/nanoplastic polymer; for example, during our analysis, PCL and PLA resulted in a particular loss of 114.07 ($C_6H_{10}O_2$), and 72.02 ($C_2H_4O_2$) respectively corresponding to monomer unit of [CL] and [LA]. The second goal was to characterize the degradation products released by the nano/microplastics in water using mass spectrometry. We considered the products released by the plastics (leaching products), produced under irradiation, and (photo)-oxidation. We have carried out this work on different polymers (e.g. methacrylate polymer, polypropylene, etc.) and for each of them, we have developed a specific analysis method. A chromatographic method with a run time of 60 minutes was developed using UHPLC-MS/MS for the identification of the transformation products of methacrylate-based expandable microspheres; the analysis shows the presence of signals from polystyrene-co-acrylonitrile (SAN) with methacrylonitrile (MA). A total of 3 oligomers of SAN, 3 transformation products (TP) each of SAN and MA, alongside 4 impurities were detected in the analyses besides the monomers. It can be concluded that microplastics release organic compounds in the liquid phase upon degradation, and most of them are byproducts of the polymerization process~~.~~ In this presentation, we will discuss various aspects of micro/nanoplastics, starting from the mass spectrometry-based identification of plastics, leachable compounds, and degradation or transformation products arising from the degradation upon irradiation using UV light and H_2O_2 under environmental-like conditions.

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O-10

Ozone (O_3) trends in Saxony (Germany) and insights from photochemical modelling

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Introduction

Tropospheric ground-level ozone (O_3) is a global air-quality pollutant that has significant impacts on human health and vegetation[1,2]. Given the importance of surface ground-level O_3, long-term observations of O_3 concentrations are of high importance to understand the O_3 formation/depletion trend in a changing environment and climate[3,4].

In this study, results of long-term trend analysis of ground level O_3 in the federal state of Saxony, Germany, are presented in different environmental site conditions, i.e. traffic, urban, rural and mountain. These trends are based on the measurements from 16 stations with long-term O_3 data (>10 years) and compared over three distinct periods: i) the entire duration of available measurement data, from 1997 or later, ii) the 15-year span from 2006 to 2020, and iii) the more recent 10 years from 2011 to 2020. In addition, also ground-level NO_x measurements at these sites were analysed. Our results highlight that O_3 pollution in Saxony has not abated and has, in fact, worsened in the last 10 years, particularly in many urban areas with dense populations despite a reduction of NO_x concentrations in all sites.

In order to understand this observation, detailed analyses of the photochemical O_3 formation and controlling effects of NO_x and VOCs were carried out with the air parcel model SPACCIM (SPectral Aerosol Cloud Chemistry Interaction Model). Only the near-explicit gas-phase mechanism MCM (Master Chemical Mechanism) was used to simulate the O_3 formation at the different environmental sites. By visualizing the station type-to-type variations in two seasonal ozone isopleths, the effectiveness of precursor controls in Saxony over past 20 years was evaluated. From these isopleths, the O_3 formation were determined to be predominantly VOC-limited regimes in traffic and urban sites during 2000 to 2019. The observed increases in O_3 levels affirm that current efforts to reduce non-methane volatile organic compounds (NMVOCs) emissions from various sources are still insufficient. Based on anthropogenic and biogenic emission data, we suggest that additional VOC emission controls should be implemented in densely populated regions in the coming years, with particular attention given to solvent usage, in order to alleviate O_3 pollution.

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O-11

Valorization strategies of plants and algae alien invasive species: new developments contributing to the circular economy

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Introduction

In last years, economic and environmental problems related to the aggressively spread of certain invasive algae and aquatic plants have been continuously increasing. *Rugulopteryx okamurae* (RO) is a species of brown seaweed originally from the coasts of the north-western Pacific Ocean, which recently invaded Spanish Mediterranean coasts [1]. *Egeria densa* (ED) is a submerged aquatic macrophyte native to South America being invasive in Spain and living in freshwater [2]. The high amount of discarded RO and ED being accumulated every year cause negative ecological and socio-economic effects. However, both species are rich in bioactive compounds, such as polysaccharides, vitamins, minerals, fatty acids and polyphenols [3]; showing enormous potential as a source of novel functional materials with specific applications.

In this work, different valorisation strategies for RO and ED species were developed according to their main chemical composition. Fatty acid extracts from RO were obtained based on microwave-assisted extraction (MAE) methodologies, including natural deep eutectic solvent (NADESs) pre-treatment to enhance the obtained yields. Several choline chloride (ChCl)-based NADESs were synthetized by using microwave irradiation. Lactic acid, urea, glycerol and thymol were evaluated as HBDs at different molar ratios to assess their ability to disrupt RO cell wall and to improve FAMEs yield. These fractions combined with polyphenols extracted by MAE from ED were successfully used to obtain alginate-based sustainable antioxidant food packaging materials to increase fruit and fish shelf-life, reducing food waste caused by spoilage. Strawberries and sardine fillets packaged in active films over 6 days of storage time were better preserved compared to the neat polymer film in terms of appearance, weight loss, color, pH, ascorbic acid content (fruit) and thiobarbituric acid reactive substances (fish). Moreover, the solid residue obtained from RO after MAE was evaluated as bio-adsorbent to remove heavy metals (Ni, Co, Cd, Pb) from residual waters, showing adsorption efficiencies higher than 90%, determined by inductively coupled plasma optical emission spectroscopy (ICP-OES). These applications can help to valorize these invasive species, also reducing the environmental problems related to its waste accumulation, contributing to the bio-circular economy.

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O-12

Development of active packaging based on activated carbon obtained from biomass waste to extend the shelf life of fruits

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Introduction

The new legislation on waste and contaminated soil covers various types of waste, including those generated in the agri-food industry, not only because of their impact on the environment but also because of the waste they entail. To encourage the circular economy, this legislation includes a tax on incineration, co-incineration and the disposal of waste in landfills, to avoid these types of final management of such waste. On the contrary, according to the European Commission and the Food and Agriculture Organization of the United Nations, one-third of food human consumption is wasted worldwide, with around 88 million tons of food being wasted in Europe, with associated costs amounting to 143 billion euros [1]. Therefore, waste valorization is necessary as an alternative to give a new use to by-products from the agri-food industry. This could be achieved by synthesizing high-added value materials such as activated carbon using such waste as a precursor. For this reason, this work focuses on the synthesis of activated carbons using biomass waste as precursor. These materials will be subsequently incorporated into polymeric matrices to have new active packaging that acts by adsorbing the ethylene emitted during the ripening process of fruits and/or vegetables, which causes their rapid deterioration [2]. The development of active packaging from activated carbon will improve the conservation and extend the shelf life of fruits and/or vegetables, contributing to the global reduction of food waste.

Activated carbons were prepared by chemical activation with phosphoric acid (H_3PO_4), which is one of the technologies that allows achieving higher yields of the final product. The synthesis of activated carbons was performed using two methodologies; the first is conventional chemical activation by impregnating biomass waste with H_3PO_4 at high concentrations (75 % w/w) and subsequent thermal treatment in an inert atmosphere up to a temperature of (or higher than) 450 ºC. The second synthesis methodology used includes a hydrothermal carbonization stage of biomass waste in the presence of a dilute aqueous solution of H_3PO_4 (25 % w/w) [3,4]. For both methodologies, the process was optimized by varying the experimental conditions (temperature, time and H_3PO_4/biomass ratio). Moreover, the effects of these experimental conditions were analyzed in terms of the activated carbon yield, textural properties and surface chemistry. The activated carbons have been characterized by physical gas adsorption, surface chemistry analysis by temperature-programmed desorption (TPD) and X-ray photoelectron spectroscopy (XPS), pH determination at the point of zero charge (pH_{PZC}) and morphology analysis by scanning electron microscopy (SEM).

The yield of the activated carbons obtained is close to 45 %. These activated carbons have specific surfaces greater than 1500 m^2/g and have been successfully incorporated into de polymer matrices. This has allowed the development of active flexible films with adequate ethylene adsorption capacity.

Acknowledgements

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O-13

Environmental risk modelling of pharmaceuticals in the water environment: Towards eco-directed prescribing in Scotland

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Introduction

Pharmaceutical pollution is a globally recognised public health and environmental issue that can negatively affect aquatic organisms, impact on drinking water quality, and contribute to the spread of antimicrobial resistance. Healthcare sustainability targets in Scotland (UK) call for improvements to prescribing and medicine use, to reduce its environmental impact [1]. In this research, we developed the first UK multi-criteria decision support tool (DST) for healthcare professionals to encourage eco-directed prescribing that presents environmental risk factors for consideration in healthcare decision-making. The probabilistic DST, based on Bayesian network models, implemented a novel decision-making framework as a blueprint to predict environmental risk and inform eco-directed prescribing for an initial list of priority pharmaceuticals, using criteria agreed with stakeholders from both the healthcare and environmental sectors. Nominal Group Technique was applied to achieve consensus on pharmaceuticals and modelling factors for the framework, working with a panel of cross-sector stakeholders representing the environment, water industry, medicines regulation, prescribing, public health, and pharmaceutical industry sectors. The priority compounds and modelling criteria were selected through surveys, facilitated discussion, and voting by stakeholders. Based on clinical and environmental considerations, four pharmaceuticals were selected: carbamazepine, clarithromycin, fluoxetine, and propranolol. Modelling factors represented the environmental exposure and hazard of the selected pharmaceuticals including: physicochemical properties, prescription and excretion rates, wastewater treatment removal rates, and dilution in the freshwater environment. The Scotland-wide Bayesian network model was produced for 40 freshwater catchments, which calculated the pollution risk score of the individual pharmaceuticals using the ratio of prescribed mass vs. mass that would not exceed the predicted no-effect concentration in the catchment. The pharmaceuticals exhibited different risk patterns, and spatial variation of risk was evident (generally related to population density), with the highest number of catchments predicted to exceed the pollution risk score for clarithromycin (probability >80% in 35 of 40 modelled catchments). Simulated risk scores were compared against observed risk calculated as the ratio of predicted environmental concentrations and measured environmental concentrations, using national regulatory and research monitoring data from the Scottish *Pharmaceuticals in the Environment* open-access database [2]. This demonstrated that the model was generally overpredicting risk, likely due to missing factors (e.g. solid-phase sorption, temporal variation), low spatial resolution and low temporal resolution of the available measured environmental concentrations. Future work will refine the framework with additional clinical and environmental factors to improve model performance, and develop electronic interfaces to communicate environmental information to healthcare professionals. This research has helped to increase awareness on the environmental impact of pharmaceuticals, and has progressed cross-sector activity to develop support tools to introduce environmental data into prescribing decision-making in Scotland.

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O-14

Photoinduced mineralisation of organic matter in the global lakes

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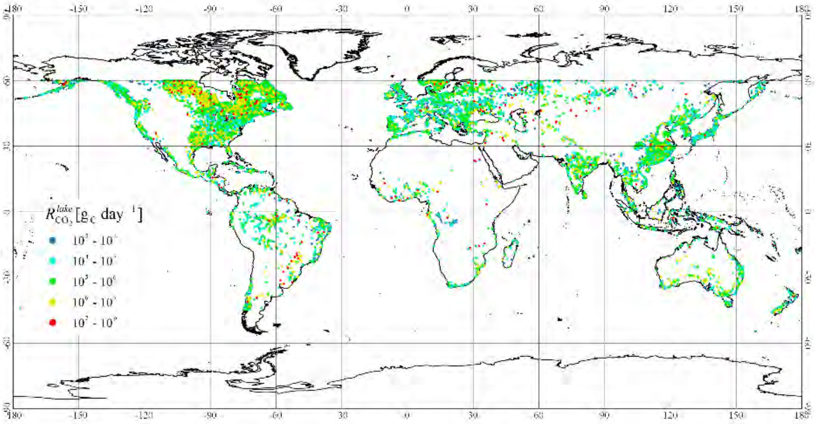
Introduction

Organic matter is the pool of diverse organic substances that occur in natural waters. Of these, a major fraction is represented by the dissolved compounds that make up the dissolved organic matter or DOM [1]. The chromophoric fraction of DOM (CDOM) is able to absorb sunlight, and the process of radiation absorption modifies organic matter with production of oxidised derivatives and volatile species such as CO and, most notably, CO_2. Photoinduced mineralisation is, in fact, the process of eventual CO_2 formation upon absorption of sunlight by organic matter in surface waters [2]. Photomineralisation is important because, although CO_2 emissions by natural waters are usually compensated for by opposite processes such as photosynthesis, possible net carbon gains or losses by aquatic environments on a global scale, if operational, would significantly affect planetary equilibria.

In this work we assessed the photochemical generation of CO_2 by lake water on a very wide (almost global) geographic scale. To do so, we combined: *(i)* Global databases of lakes, which provide information about geographical location, depth, surface area, and the dissolved organic carbon (DOC) [3]. *(ii)* A monochromatic approximation to photoinduced reactions [4], which allows for a considerable simplification of the otherwise very complex multi-wavelength calculations (including most notably the absorption of sunlight by CDOM along the water column), with negligible loss in accuracy. *(iii)* A quasi-global assessment of the spectral photon flux density of sunlight reaching the ground [5].

The map below reports the photoproduction of CO_2 (yearly average) by lakes in the latitude belt from 60°S to 60°N. Two considerations can be made: *(i)* around 50% of the total CO_2 generation is accounted for by the seven most productive lakes (Caspian Sea, Baikal, Superior, Michigan, Huron, Erie, Malawi); *(ii)* six out of the seven lakes that produce the most CO_2 are located between 30°N and 60°N latitude.



Acknowledgements

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O-15

The need of analysis of new substances in drinking and bottled waters

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Introduction

Water plays key roles in our lives. One of these is its consumption, either in the form of tap water or as bottled waters. Both types of water have certain qualities and limitations, depending on the consumer's health, its financial situation or just consumer’s preferences [1]. Therefore, it is necessary to have a more complete knowledge of about their composition, origin, production, and storage methods. The cost of routine water monitoring is high, and its scope and the results obtained do not fully reflect data on its quality. The subjects of research are mainly substances and elements that have been known for a long time, the lists of which are included in the relevant regulations. Unfortunately, we sometimes forget about new hazards and substances that we already know may be present in them, but are not yet regulated.

Systematically, as new toxicological data are obtained and development of analytical chemistry, regulations are changing regarding requirements for tap water, as well as bottled water. The changes affect both the types and permissible contents of the analytes to be determined [2]. In addition to routinely determined organics and organic substances, many papers have been published in past years on the need to determine new substances have been published [3].

These include nano- and microplastics, nanomaterials, pharmaceuticals, flame retardants, contrast agents used in medicine, personal care products, pesticides and many others. In 2020, a new European Directive on the quality of drinking water began to be implemented in EU countries [4]. Compared to the existing regulations, the scope of testing is broader, among others, by the need to determine uranium, bisphenol, halogenoacetic acids and other substances such as microplastic, nonylphenol and β-estradiol from observation list. Taking into consideration development of analytical chemistry, and new toxicological data, the list of new substances that will be determined in drinking water is bound to expand. Analytical chemistry is ready for this, but are we prepared for it in terms of the necessary costs, both financial and environmental? These activities generate additional costs (including environmental costs) [5], but it is necessary and should be introduced systematically in accordance with the principles of green chemistry. Globalization, new technologies, climate change, over-consumption and emergencies such as the recent SARS-Cov-2 pandemic make it necessary to expand research in this area and update existing knowledge. The question is to what these factors affect the quality of both drinking waters? Are new substances that have not yet been mentioned in the recent regulations present in them, and if so, in what concentrations? Does it depend on where their waters are produced (geological and environmental conditions), how they are stored (time, types of packaging), and can they have a significant impact on consumer health?

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O-16

Environmental emergencies: nanoplastics and microplastics, impacts and solutions

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Introduction

The prevalence of nanoplastics and microplastics as pollutants in aquatic ecosystems is drawing significant attention. The prevalence of nanoplastics and microplastics in aquatic ecosystems, resulting from both primary and secondary sources, creates a milieu of contaminants with potentially adverse effects on the ecosystems and the organisms therein [1]. As nanoplastics and microplastics exist in micro-level to nano-level sizes, they are virtually impossible to remove once released into the environment. Due to these characteristics, microplastics pose potential hazards to humans and the environment. There is a pressing demand for the advancement of novel materials and innovative technologies geared toward effectively eliminating emerging organic pollutants, such as nanoplastics and microplastics [2]. A unique hybrid technology was developed for the removal of specific contaminants from wastewater. Reactor testing was performed using model water samples contaminated with pharmaceuticals and microplastics. Different hydraulic retention times, concentrations of pollutants and dissolved ozone were tested. Liquid Chromatography-Mass Spectrometry, solid phase extraction, surface area and porosity, analytical tools were used to monitor the treatment efficiency and remaining sorption capacity of the spent adsorbent. The combination of advanced oxidation and adsorption processes was found to be the most effective, with the highest 90-99% and 89-95% pharmaceuticals and microplastics contaminants removal efficiency from the model wastewater.

Acknowledgements

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O-17

Modern smoking – vaping – inhalation of other volatile organic compounds (VOCs) besides nicotine

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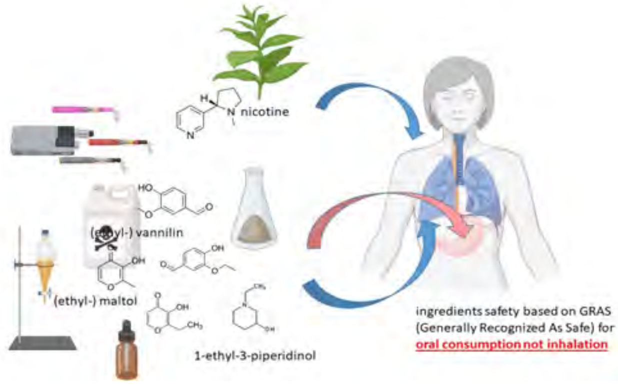
Introduction

Tobacco product regulations, which vary by country or region [1,2] generally require electronic nicotine delivery systems (ENDS) packaging to include the following: nicotine content, warnings (e.g., "an addictive substance"), product labelling, manufacturer information (i.e. batch number, expiry date,..) and an ingredient list, containing flavorings, sweetners, solvents, etc.. These last compounds are (according to manufacture companies) claimed safe based on GRAS regulatory status (generally recognized as safe for food – oral consumption). However, this statement cannot apply for the same substances when they are inhaled [2]. Another loophole arises from the U.S. Food & Drug Administration (FDA) regulations, which ban most flavours in tank and cartridge-based e-cigarettes, whereas disposable e-cigarettes (vapes), popular among youth, remain largely unregulated due to ambiguities in defining a cartridge [1].

Our study included 8 flavoured vapes purchased in Ljubljana, Slovenia, in November 2023. All vapes, were labelled with a nicotine content below 20 mg/mL, packed in 2 mL cartridges, providing 550–600 puffs. By using gas chromatography mass spectrometry (GC-MS), vape liquids (diluted 1:100 with hexane) were analysed in triplicates. Volatile compounds (VOCs), identified by comparing mass spectra to a reference library (NIST02), that account for more than 1% of total sum of peaks' areas (more than 0.3 mg/mL expressed in nicotine equivalents) were highlighted and those exceeding 5 mg/mL were analysed in detail. As Omaiye et al. (2022) found in their study (1 mg/mL volatiles in vapes); the list of volatiles that stood out in our study included: maltol, ethyl maltol, vanillin, ethyl vanillin [3]. Besides those, also benzoic acid, 1-ethyl-3-piperidinol, and (Z)-N,N-dimethyl non-7-enamide were of higher concentrations. Ethyl maltol and vanillin were linked to free radical formation, cytotoxicity, and inflammation. Benzoic acid, commonly used to adjust nicotine pH, raises concerns as it generates reactive oxygen species (ROS) and benzene, a known carcinogen. Vanillin and ethyl vanillin, safe for oral consumption, show cytotoxic effects when inhaled. For other compounds like 1-ethyl-3-piperidinol, only limited studies are available that show possible health risks from second-hand vaping. Our study is just one of many worldwide highlighting the dangers of the unregulated vape market.



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O-18

Synthesis, evaluation of halogenated BPA and paraben compounds

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Introduction

Environmental chemicals with widespread human exposure such as bisphenol A (BPA), endocrine-disrupting chemicals (EDC), may play an important role in de-regulating normal metabolism.[1] BPA is detected in various environmental matrixes (food, water, dust), and then generates public concerns regarding its health risks, inducing pathologies as disrupted development, altered reproductive toxicity and cancers. [2-3]

Our research focused on BPA, its chlorinated derivatives (Cl_xBPA) formed during the water chloration, but also brominated derivatives of BPA (Br_xBPA).[4-5] BPA and its halogenated derivatives were described as agonists of estrogen receptors (ERs) and proliferator peroxysome activator receptor © (PPAR©) and antagonists of the androgen receptor (AR). Parabens, used as preservatives, were also described as ligands of ERs and AR. Like BPA, parabens afforded chlorinated, brominated analogs, which were very limited studied. [6-7]

We firstly synthesized halogenated BPA and parabens derivatives. In a second time, we determined the activities of chlorinated and brominated derivatives (for both bisphenols and parabens) for ERs, AR, PPAR©, pregnane X receptor (PXR) and constitutive androstane receptor (CAR) using bioluminescent reporter cell lines. Finally, the effect of chlorinated and brominated derivative bisphenols/parabens were studied using MCF-7 breast cancer cells (which express a large panel of the nuclear receptors mentioned above) and the XCelligence system, which allows a real-time follow-up of several cellular properties including proliferation, adhesion and migration for several days. Complementary experiments were performed such as migration and invasion tests (Transwell) and identification of biomarkers through real-time PCR and/or western blots, together with the use of co-culture (with pre-adipocytes and adipocytes) systems to study the co-influence of 1) the derivatives and 2) the microenvironment, on the acquisition of stemness and chemoresistance.

Acknowledgements

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O-19

Isolation of cellulose from soybean hulls: efficiency and sustainability of different strategies

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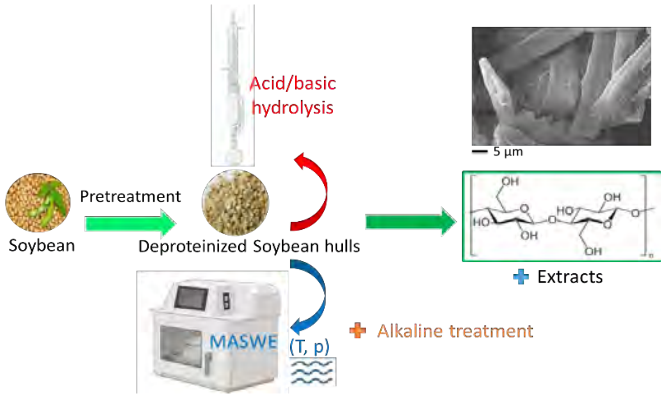
Introduction

Recently, biopolymer extraction from (waste) biomasses has been considered a valuable approach to obtain sustainable compounds usable for different purposes, avoiding the indiscriminate dispersion of putrescible matter in the environment or the costs of waste disposal. Indeed, agro-industrial residues are rich in components exploitable as new raw materials in several application fields, such as food packaging, bioplastics, and in the biomedical and water treatment sectors [1,2]. Such wastes are mainly composed of cellulose, hemicellulose, lignin, polyphenols, starch, etc., depending on the starting crop [2].



Traditional extraction routes of these components often employ multistep processes in acidic/alkaline conditions to promote hydrolysis and their consequent isolation from the matrixes [3], which are pretty far from the green chemistry fundamentals, which suggest avoiding polluting, corrosive and hazardous reactants.

Cellulose, in particular, is one of the most abundant carbohydrates in nature and a versatile compound, easily modifiable to create a plethora of innovative materials. In this research work, we focused our attention on the optimization of its green isolation from soybean hulls already deprived of peroxidase enzyme. Soybean hulls are one of the by-products of soybean (*Glycine max*) crushing and, to give an idea of the quantity involved, soybean global production is around hundreds million tons [4]. The classical cellulose isolation through acid-basic hydrolysis was compared with that performed by Microwave-assisted Subcritical Water Extraction (MASWE). MASWE technique has (i) fast heating, (ii) increased selectivity and yields and (iii) high thermal efficiency as the main advantages [5]. Both the obtained cellulosic samples and the liquid extracts have been characterized (SEM, TGA, DSC, FT-IR, NREL, phenolic content) to select the best extraction conditions. Overall, the outcomes from cellulose isolation ability and final material characterization revealed that the coupling of MASWE operated at 180 °C with an alkaline treatment was the most efficient procedure.

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O-20

MICROPLASTICS from tires. An emerging concern

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Introduction

Microplastic pollution is a main hot topic for many agencies and bodies such as the ECHA (Europe) and the US EPA, being nowadays a recognized public concern. Tire particles is a major source of microplastics in the environment since the particles produced incidentally by vehicles are the second source of microplastics reaching the environment. Crumb rubber from end-of-life tires employed in sports pitches and playgrounds is the first source of microplastics in the environment, being also a main issue for ECHA and other agencies [1]. This material is a complex mixture of hazardous chemicals, some of which are very well known such as PAHs or heavy metals [2,3]. However, other emerging contaminants such as those belonging to the p-phenylenediamine family (PPDs) have received little attention and only very recently they emerged as environmentally hazardous substances [4,5]. In this way, not only the microplastic itself pollutes the environment but also all the hundreds of chemicals included in this complex mixture. In this talk, the presence of a high number of classical pollutants but also of new emerging contaminants such as 6PPD and its by-product 6PPDq and of other additives will be shown, not only in the tire particles and crumb rubber but also in environmental, biological and food matrices. Different advanced extraction and microextraction approaches in combination with LC-MS/MS and GC-MS/MS will be proposed to accomplish analyses [5-7]. The application to a wide range of real samples, including biaccessibility [8] and photodegradation studies, will contribute significantly to the knowledge of the global impact of microplastics issued from recycled tire crumb rubber, from both an environmental and human health perspectives.

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O-21

Electrochemical monitoring of BIT photo(catalytic)degradation

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Introduction

Cleaning agents play important role in our everyday life, since with a safe and proper use we can effectively remove a large portion of dirt. Although surfactants are one of the main components of detergents, recently a serious source of the pollution of municipal wastewaters coming from dishwashing is the added biocides. Benzisothiazolinone (BIT), as one of them, belongs to the isothiazolinone family, known for their potent antimicrobial and antifungal properties [1].

BIT is persistent in the environment, with a half-life of more than 30 days, and can be transported through soil and water pathways. Conventional wastewater treatment plants efficiently remove isothiasolinones at low concentrations, but at higher concentrations ozonation and other AOP methods are proposed.

In our study we investigated the photo(catalytic) degradation of BIT using ZnO which was proved to be efficient photocatalyst for removal of some other pollutants [2]. For in-situ detection of BIT we need fast, reliable tools for what the electrochemical sensors are good candidates [3,4].

ZnO photocatalytic and photolytic (without ZnO) experiments were performed in photoreactor equipped with polychromatic low-pressure mercury lamps (1.6 mW/cm^2 of UVA (300 - 400 nm)) as well as with UVC germicidal lamps (254 nm). In the case of photolytic experiments, BIT aqueous solution was irradiated for 120 min in the presence and absence of oxygen, while photocatalytic degradation of BIT aqueous solution was carried out under constant air flow. BIT removal was traced using electrochemical sensors based on screen-printed electrodes (SPE) with conductive working electrode, quasi Ag reference electrode and Pt counter electrode. In this work, carbon nanoparticle based working electrode was used in the PBS buffer (pH 7,4) and square wave voltammetry (SWV) was applied between 0.2 V and 1.1 V with a potential step of 10 mV, amplitude of 30 mV and frequency of 10 Hz to detect the BIT oxidation peaks. The BIT oxidation peaks at 0.6 V vs. quasi-Ag were detected in all cases and the height of the peak (current) was correlated to the concentration of the UV degraded BIT. ZnO photocatalytic treatment proved to be the most efficient at removing BIT, followed by photolytic treatment by UVC and UVA, respectively. In both ZnO and UVC samples, the BIT concentration was below the LOD after 45 minutes, while the UVA treatment did not remove the pollutant even after 180 minutes. The degradation of was proved by classical analytical method (HPLC-DAD) and some degradation products (benzamide, salicylamide) have been tentatively identified by GC-MS.

Acknowledgements

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O-22

PFAS removal by minerals and advanced removal by tailored polymer-mineral composites

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Introduction

Per- and polyfluoroalkyl substances (PFASs) are emerging pollutants due to their persistent nature in the environment and potential adverse effects on ecological systems and mammal's health. Despite various water treatment methods available for PFAS removal, no single approach provides a comprehensive solution for all PFAS contaminants [1]. We suggested that adsorption-based technologies utilizing metal oxides and advanced tailored polymers composite can offer high efficiency in the removal of micropollutants, specifically PFASs.

We aim to remove an array of PFASs by simple oxides and tackle those PFAS which are not removed (probably the short chains) by synthesising advanced tailored polymer mineral composite. Initially, we assessed the removal efficiency and adsorption mechanisms of PFASs using different oxide sorbents. We observed that the adsorption capacity and affinity of the PFAS molecules were influenced by the surface charge of the oxides (positive, neutral, or negative), showing that PFAS molecules exhibit a higher affinity towards oxides with increasing positive surface charge.

Testing the adsorption kinetics revealed distinct behaviours for PFOS and PFOA. PFOA exhibited particularly faster adsorption kinetics (k) and faster desorption rates (k') compared to PFOS, indicating a more rapid binding with the carboxylic acid head of PFOA over the PFOS with the sulfuric acid head but slower desorption of the later. Interestingly, despite the faster kinetics of PFOA, PFOS showed a higher equilibrium affinity for the oxides over PFOA. The higher affinity attributed to the stronger acidity of the sulfuric acid head compared to the carboxylic acid head of PFOA. The obtained adsorption isotherm hinted stepwise adsorption as the contaminant concentration increased. We suggest that the stepwise adsorption indicates the formation of multilayers of PFAS molecules atop a monolayer of adsorbed PFASs. We tested the removal of several PFASs from ground water and found (like many other studies) that while the removal of the 8-carbon chain molecules high, as the chain length decreases the removal decreases as well.

Since short chain PFASs are more challenging to remove, we synthesized advanced tailored polymer-mineral composites with various organic functional groups. We suggest that in addition to the composites' charge, the physical structure of the composite also plays a critical role in PFAS removal. We evaluated three types of synthesize composites—grafted monomer composites, adsorbed polymer composites, and grafted polymer composites with different lengths and brush densities. The results also showed that long-chain PFASs, and more importantly, short-chain PFASs, were more effectively adsorbed by grafted polymer composites, specifically the grafted composite with the long polymer and low brushes density, demonstrating a 1.6-fold enhancement in the removal of a 5-carbon chain PFAS with a carboxylic head, compared to adsorbed polymer composites and 2.4-fold enhancement compered to grafted monomer composites. We suggest that the structure complexity, caused by the long polymers intermolecular binding, creating new available binding sites and the lower brush density minimizes steric effect.

Yet these metal oxide and advanced composites do not allow complete PFAS removal, but it give us an insight into the binding mechanisms and better understanding the chemical and physical structure role in the removal of PFASs.

Our ongoing research aims to evaluate these oxides and advanced polymer-mineral composites in column studies to assess their synchronize performance on a larger scale.

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O-23

Resource recovery from wastewater with biochar: quality assessment and phosphorus fractionation

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Introduction

Phosphorus (P) is a crucial element for global food security, with the demand for P from non-renewable resources growing rapidly in the last 100 years. As phosphate rock resources are depleting, new management tools for environmentally friendly P fertilisers and sources are needed. Sewage sludge (SS) and biosolids are considered secondary P resources with potential for mitigating the demand for mineral P sources. Additionally, SS disposal on land can pose risks to surface water and soil quality, i.e., through the addition of potential contaminants [1]. Thus, conversion of SS to biochar (SSB) achieves a dual purpose through solid waste repurposing and pollution elimination, while well align with the concept of a more circular economy and carbon neutrality (as biochar is also a stable solid form of carbon) [2]. P is the nutrient present in the highest concentrations in biochar. P is present in SSB in several organic and inorganic fractions with different degrees of stability/solubility.

This work explored the P solubility and fractionation using different chemical extractants (i.e., water, 2% citric acid, 0.5 M $NaHCO_3$, 0.6 M HNO_3, microwave H_2O_2/HNO_3 extraction) from six different SSB. Additionally, the proximate analysis coupled with instrumental characterisation (CHN, SEM-EDX, BET, FTIR, TGA, XRD and XPS techniques), and leaching experiments (for organic contaminants and heavy metals) determined the biochars stability in simulated soil environments.

Instrumental characterisation showed that adsorption was dominated by metal-phosphate precipitation and inner-sphere complexation onto metal ligands (mostly aluminium and iron). The total P concentrations (expressed as P_2O_5) obtained from microwave H_2O_2/HNO_3 extraction ranged from 5.8% to 11.7%. The water extraction showed poor water solubility (<1%), while the 0.5 M $NaHCO_3$ (simulated alkaline soil condition) and 2% citric acid (simulated acidic soil condition) comprised <10% and >30% of total P, respectively. Despite the limited readily available P, all the biochars can be used as a slow-release P fertiliser with long-term effect which is a desirable characteristic of fertilisers applied in soils with high P deficiency. The extraction with 0.6 M HNO_3 (simulated industrial leaching) showed that almost 100% of the total P can be leached out from the biochars, which suggest a great potential for these materials as P sources in different industrial sectors dependent on P (i.e., drink/food, steel and chemical). Taking into the consideration legislative limits for heavy metals set by the World and European Biochar Certificates, results indicated only trace levels of Pb, Cu, Cd, Ni, Cr, As and Zn in all biochars with extractants realistic for soil conditions (e.g., water, 2% citric acid and 0.5 M $NaHCO_3$). Microwave H_2O_2/HNO_3 and 0.6 M HNO_3 extraction immobilised higher levels of Cd, Pb, Zn and Cu, however these eluents simulated harsh acidic environments which are unlikely in nature. Overall, the results showed the great stability of these metals within the SSB structure. Organic analysis showed trace levels of PAHs and PCB, while PFAS/PFOS were below the detection limits, which also indicated the ‘relative’ purity of the SSB.

This study enabled to understand the P fractionation in the biochars and its quality, which could help to design future pot and long-term field trials in relevant environments.

Acknowledgements

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O-24

Promoting the self-immobilisation of activated carbon for enhanced adsorption of organic micropollutants

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Introduction

The occurrence of trace organic micropollutants in drinking water is alarming, owing to the possibility of harmful risks to human health. Water treatment technologies have to be developed in order to combat the ineptitude of conventional treatment processes. Carbon materials can be used as efficient adsorbents or catalysts for the removal of a variety of chemicals present in water. In particular, activated carbon (AC) derived materials have been thoroughly investigated for the adsorption of pharmaceutical compounds [1].

In this work, we propose the incorporation of nitrogen groups onto the AC matrix and assess the self-immobilisation of these materials onto three-dimensional alumina beads to overcome the adsorbent separation step and to allow continuous mode operation. The AC was functionalised with nitrogen groups by the addition of urea in the synthesis process with different ratios (so-called *x*U@AC, where *x* stands for the quantity of urea per gram of AC), following a previously studied heating procedure. The materials were applied in continuous mode for the adsorption of venlafaxine and diclofenac – pharmaceuticals commonly found in surface waters.

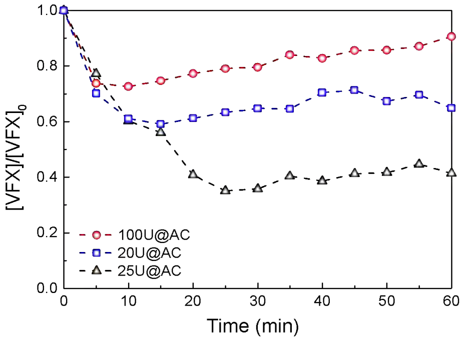

Figure 1. Venlafaxine (VFX) adsorption by AC-loaded alumina beads ion a packed-bed flow reactor under continuous operation.

Moreover, the catalytic ability of AC was assessed for the oxidation of organic molecules present in water in the presence of spike hydrogen peroxide, promoting catalytic wet peroxide oxidation (CWPO). The CWPO mechanism was employed for the regeneration of spent adsorbents. Reuse experiments were conducted to prove the applicability of this system.

Acknowledgements

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O-25

Heavy metals levels in the close neighbourhood of the industrial waste landfills in Lodz region

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Introduction

Landfilling is recognized as the oldest method of solid waste disposal. It also can pose a serious threat to the environment. This method is mostly chosen due to the apparent simplicity of operation and low costs. The landfill sites are often described as reactors of biological, physical, and chemical transformations, which may undergo in the stockpiled wastes. As a result of the ongoing processes, there is a risk, despite the undertaken remedial actions, of the release of some gases that may contribute to the local spontaneous combustion of wastes. Moreover, these places can face the problem of the leaching of waste components into the underneath soil and groundwater. Leachate, being an important source of environmental pollution, is defined as a liquid from the waste landfilled, which is generated under the influence of the amount of moisture in the landfill site and as a consequence of the chemical and physical reactions. Heavy metals are one of the most important pollutants in landfill leachate, and plants and soil near the landfill can be contaminated by them [1-2].

In this work, we attempted to determine the content of some selected toxic elements in samples taken in the close neighborhood of the industrial waste landfills and compare them with the results of the same type of samples originating from the control sites to investigate the degree of pollution caused by the leachate in the environment around the landfills. In the Lodz region, in the city of Zgierz, there are several landfills containing the waste products from industrial activity. Unfortunately, for many years there was no interest in the regular inspections of the area, which also affected some illegal stockpiling of wastes of unknown origin. Material of soil and plants was collected from the sampling points situated in the vicinity of the waste landfills in Zgierz in the years: 2023 and 2024. Most of the wastes stored there are remains of the Boruta Factory. The studied area is covered by four different landfills. The hazardous wastes landfill contains over 40 tons of post-production waste from the former "Boruta Plant", stored in containers and barrels from the years 1995-2006. Moreover, in the years 2012-2015, huge amounts of waste of various origins, including municipal waste, were illegally deposited at this landfill. A landfill of post-production furnace ashes and gypsum, the so-called “dry landfilled”, has existed since 1960. After the end of the landfill's operation in 1986, gypsum and calcium salt from acid production were stored for about 10 years. It is estimated that since 1990, approximately 1,500 tons of waste have been added annually. The third location is the neighborhood of the private owner area where undefined wastes were stored there. The oldest industrial landfill is located directly on the river Bzura. It is estimated that until it was closed in 1995, it had been in operation for 80-90 years. Due to the long period of time, the volume of stored waste is not known. Since 1990, when waste recording began, the annual revenue was approximately 270 tons per year. Currently, the landfill area is covered with dense vegetation and numerous trees. The main aim of this work was to verify the possible influence of industrial waste landfills on the level of chosen heavy metals determined in soil and plant material. This study was conducted in different locations in Zgierz and Łódź cities and soil and plant samples were prepared according to a specific protocol. Before the multielement analysis, dried samples were treated with the mixture of concentrated acids HNO_3 and HCl (soil) or HNO_3 and H_2O_2 (plant material) and decomposed in a closed-pressure microwave digestion system. After the mineralization extracts were centrifuged and the extractable content of chosen elements was measured by the Inductively Coupled Plasma Optical Emission Spectroscopy technique (ICP-OES) iCAP7400, (Thermo Scientific). Even though all samples in Zgierz were collected in the closest vicinity of the waste landfills (not directly from the waste disposal places) and most of the area studied was covered by the forest, the obtained results for material from Zgierz were much higher in comparison with the data gathered for the samples from the control cites, which all suggests that studied area is highly affected by the presence of the waste disposal places.

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OY-01

Bifunctional carbon-supported Pd-based catalysts for the sustainable production and storage of H_2 attained by formic acid-bicarbonate couple

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Introduction

Formic acid (HCOOH) has emerged as a very interesting Liquid Organic Hydrogen Carrier (LOHC) because of its high volumetric hydrogen density, low toxicity and high stability, which makes it a potential solution to the problems of hydrogen storage. Moreover, it is involved in a H_2 production and storage system based on an ideally carbon-neutral cycle, formed by the dehydrogenation of formic acid and the hydrogenation of CO_2. However, the hydrogenation reaction is much more challenging than the dehydrogenation of HCOOH due to its unfavourable thermodynamics (CO_2 (g) + H_2 (g) → HCOOH (l), ΔG_{298K}= 32.9 kJ·mol^{-1}) [1]. The most straightforward approach to overcome the thermodynamic limitation is to conduct the reaction in the liquid phase using alkaline additives such as bicarbonates, amines, and hydroxides [2].

In this work, Pd-based catalysts, with different compositions of the metal nanoparticles and supported on activated carbon derived from biomass residues, were prepared and assessed in the H_2-formate interconversion via formic acid dehydrogenation and bicarbonate hydrogenation reactions. These developed materials were characterized using different physicochemical techniques such as X-ray photoelectron spectroscopy (XPS), Transmission Electron Microscopy (TEM) and Inductively Coupled Plasma Optical Emission spectroscopy (ICP-OES). The results of the catalytic tests for both reactions are shown in Figure 1. Considering the results of both reactions, and that the hydrogenation of sodium bicarbonate is a more hindered reaction, we obtained that the catalyst with the bimetallic composition of Pd-Ni was the most promising among those investigated. Successive stability tests were carried out with that catalyst and it displayed an interesting performance.

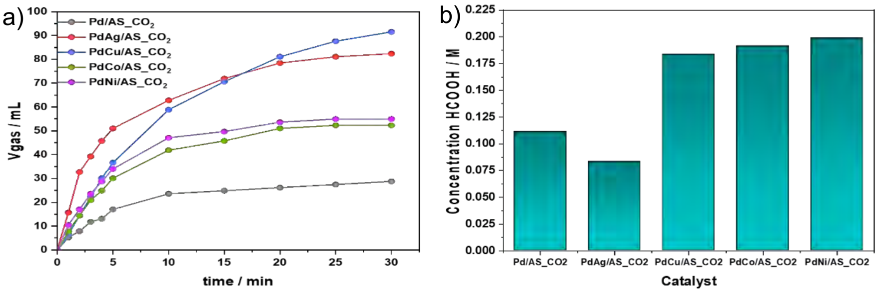

Figure 1. A) Volume of gas generated by each catalyst in the dehydrogenation reaction at 75 ºC. B) Concentration of HCOOH formed by each catalyst in the hydrogenation of sodium bicarbonate at 100 ºC.

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OY-02

Biotechnological valorisation of acid mine drainage: Seaweed as a green tool for rare earth elements recovery

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Introduction

Technology-critical elements (TCEs) such as rare-earth elements (REEs) are considered critical raw materials for many emerging technologies[1]. Mining remains the largest source of TCEs, and the waste/pollution resulting from mining activities pose serious environmental hazards. Acid mine drainage (AMD) is harmful to the environment and negatively affects marine and terrestrial ecosystems due to its considerable amount of toxic elements, its acid character and persistence (thousands of years)[2]. Yet, AMD has a prominent concentration of TCEs, which recovery would promote the valorisation of AMD and the recycling/reuse of mining waste as secondary source of these critical raw materials[3]. Among potentially low-cost sorbent materials, seaweed are considered a greener, cost-effective and environmentally friendly alternative with a high potential for recovering TCEs from aqueous solutions[4].

The present work investigates for the first time the seaweed potential to remove, concentrate, and recover TCEs from raw AMD, while improving water quality, thus contributing to Sustainable Development Goals No. 6, 12 and 14.

AMD samples were collected from a closed Portuguese mine and characterized using Inductively Coupled Plasma Mass Spectrometry, selecting the elements of economic interest. The results revealed the presence of concentrations in the order of 300 – 1000 µg/L of ΣREEs, Co and Ni. A comparative study of living (bioaccumulation) and dried (biosorption) seaweed species (*Ulva* sp., *Gracilaria* sp. and *Fucus* sp.) under the original physicochemical conditions of AMD showed that bioaccumulation was the most efficient process (REEs removal between 32-44%, 63-75%, 17-29% respectively), yet *Gracilaria* and *Ulva* species also removed over 60% of Fe. Adjusting the pH of AMD with NaOH successfully separated unwanted elements with minimal REEs loss. The seaweed dosage (0.08-0.3 ratio V/m) was evaluated for both *Ulva* and *Gracilaria* species. Overall, *Gracilaria* sp. stood out and accumulated up to 274 µg/g of ΣREEs, corresponding to bioconcentration factors between 414-1470. FTIR and SEM-EDS analysis identified sulphonate, carboxyl and alkyne groups as key in binding elements to *Gracilaria* sp. biomass.

Overall, these results support the use of living seaweed as the basis of an efficient, greener, and sustainable technology, easily incorporated in the current passive treatment systems, to value AMD-containing REEs, and other TCEs.

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OY-03

Bisphenols extraction from water samples employing a natural deep eutectic solvent-based liquid-liquid microextraction technique

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Introduction

Recently, there has been increased interest in the use of natural deep eutectic solvents (NADESs) in microextraction processes, in part due to their components are originated from nature, their low toxicity, low vapor pressure, high thermal stability, simplicity of synthesis at room temperature, high purity and low cost [1]. On the other hand, bisphenols (BPs) are a series of synthetic organic compounds that include several analogous structures such as bisphenol A (BPA), bisphenol S (BPS), bisphenol AP (BPAP), bisphenol AF (BPAF), bisphenol F (BPF), among others. These compounds are employed in the plastic industry for food containers and packaging materials, and coatings on metal cans and bottle tops. Therefore, BPs can migrate from food packaging and there has been growing concern about BPs release into environmental matrices (i.e., surface waters).

The aim of this study is to develop a new method for determining 5 bisphenols (i.e., BPS, BPA, BPAP, BPAF and BPF) in water samples using a NADES. Decanoic acid:DL-menthol in a molar ratio of 1:2 is used as an environmentally friendly extractant for extraction and preconcentration of BPs using dispersive liquid–liquid microextraction before liquid chromatography coupled with a diode array detector (LC-DAD). The method has been evaluated under optimized conditions (i.e., NADES volume, 50 µL; sample pH, 7; extraction time, 3 min; centrifugation speed, 2000 rpm; and centrifugation time, 2 min), obtaining good linearity with correlation coefficients ranging between 0.993 and 0.999 (N = 8).

The relative standard deviation values range range from 4 to 19%, and the detection limits are between 1.5 and 3.5 µg/L. Recovery tests carried out on different water samples (i.e., mineral and river water) provide relative recoveries between 70 and 118%. In addition, a migration study with polycarbonate bottles has been carried out, as well as the analysis of water from different sources such as bottled mineral water, river water and water from companies that supplied bottled water directly to consumers. Finally, the greenness of the method has also been evaluated.

Acknowledgements

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OY-04

Chitosan, gelatine and cellulose based hydrogels for the removal of potentially toxic elements from aquaculture water: a comparative study

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Introduction

In the last seven decades' total fisheries and aquaculture production has significantly expanded with an annual growth rate of 3.3%. Recent FAO reports highlighted the importance of aquaculture contribution to fighting poverty, hunger and malnutrition as more than half of aquatic food are farmed [1].

In this context a central theme is the preservation of the healthiness of water resources which may be subject to contamination due to a wide range of anthropic activities. Among the water contaminants, potentially toxic elements (PTEs) represent a well-known problem for ecosystems safety and for human health [2]. Indeed, PTEs are not biodegradable and can bioaccumulate in fishes with a consequent biomagnification along the food chain [3].

Adsorption is one of the most efficient techniques for PTEs' contaminated water remediation and offers many advantages including fitting well into the circular economy paradigm, allowing the development of materials as sustainable as possible.

In this study three different hydrogels were synthesized starting from cellulose and alginate (HY-ACMC), gelatine (HY-MGEL) and chitosan (HY-MCHI) obtained, or obtainable, from agro-industrial waste. They have been characterized and tested for the removal of a mixture of 7 PTEs (Pb, Zn, Cu, Cd, Ni, As and Hg) from both ultra-pure and aquaculture spiked water. Their adsorption capabilities as a function of the contaminants initial concentration and the solution pH have been studied. Furthermore, their efficiency after multiple cycles of adsorption and successive regeneration with Na_2EDTA has been investigated.

Although all tested materials showed promising removal capabilities also in actual waters, HY-ACMC has proven to be the most effective for single-cycle remediation treatments as it maintains high performance in all the studied conditions, however proving unstable to regeneration. On the other hand, regeneration with Na_2EDTA improves HY-MCHI efficiency granting its prolonged employment over time. However, considering both performances in real water samples and reusability results, HY-MGEL seems to be the most reliable material for multiple cycles of water remediation treatments. Finally, the end-of-life impact of the hydrogels was studied *via* biodegradation experiments by burial in compost. The results show a non-significant increase in background values for the majority of the contaminants studied, suggesting that by maximizing desorption efficiency, biodegradation can be considered a promising way to close the life cycle of these materials.

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OY-05

Innovative electrochemically controlled liquid-liquid microextraction (EC-LLME) using hydrophilic deep eutectic solvent for efficient heavy metal extraction from edible oil samples

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Introduction

Heavy metals are naturally present in the environment, and at appropriate concentration levels, they are essential for normal physiological functions. For example, a deficiency in nickel can hinder growth and lead to increased levels of urea and glucose in the blood, resulting in liver damage. However, excessive exposure to heavy metals can cause various health problems, including asthma, allergic reactions, and severe conditions such as different types of cancer [1]. Human exposure to these toxic elements frequently occurs through the consumption of contaminated water or food. In order to help mitigating potential health risks, it is essential to develop sensitive and accurate analytical methods to monitor heavy metal concentrations in these samples.

To address this issue, the present work introduces a novel, sustainable approach by combining a liquid-phase microextraction (LPME) technique with electrochemistry for the separation and preconcentration of selected analytes (specifically Cd, Cu, Fe, Ni, and Pb), followed by detection using inductively coupled plasma optical emission spectroscopy (ICP-OES). Specifically, electrochemically controlled liquid-liquid microextraction (EC-LLME) is utilized to improve metal extraction efficiency while minimizing reagent consumption, waste generation, and energy use.

In this study, a hydrophilic deep eutectic solvent (DES) composed of choline chloride (ChCl) and ethylene glycol (EG) in a 1:2 molar ratio was employed to extract heavy metals from edible oil samples. Following the optimisation of key parameters through multivariate analysis, the method exhibited a notable enhancement in heavy metal extraction. Furthermore, the limits of quantification (LOQ) obtained with the proposed methods ranged from 0.3 to 5 $\mu g\ L^{-1}$. Additionally, the trueness was evaluated through recovery experiments in real edible oils samples, demonstrating recovery values within the range of 94–103%. This innovative approach, which combines microextraction with electrochemistry and incorporates a hydrophilic DES, presents a promising alternative to traditional sample preparation methods.

Acknowledgements

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OY-06

Towards agrochemical leachate prevention through application of flow synthesised chitosan-apatite fertiliser

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Introduction

Flow chemistry is best when opening ‘novel process windows’[1], and one of six NPW paths is “new chemical transformations”. Flow chemistry has large impact on nanomaterial synthesis as this is particularly mixing-sensitive. A gap still is to produce nanomaterials of a superior performance in material design and functionality; in the sense of above NPW path. Here we report about the flow synthesis of fertiliser capsules with a chitosan coating around a chitosan/citric acid matrix that comprises dispersed phosphorus (P) nanoparticles (apatite). These capsules are connected *via* a chitosan string, resembling necklaces, adding a 3rd hierarchy in scale (3D) to the two hierarchies of coating and matrix. The strings of necklaces were woven into a mesh-like structure, adding a 4th hierarchy scale (4D). A stack of those meshes has potential to enable precise and uniform fertiliser release over a soil volume. Controlled-release fertilisers of macronutrients as P are critical for agricultural efficiency to reduce non-point source pollution causing by nutrient runoff/leaching. Using combined sheath and segmented flow in a water/oil system, the capsules had a consistent composition and morphology with an average content for phosphate and potassium of 24.5 wt% and 7 wt%, respectively. The resulting fertiliser exhibited slower nutrient release and extended lifetimes in aqueous media with 62 days in mild acidic solution, against 2422 days in deionised water. Soil column experiments demonstrated a low leaching loss for the sheath-flow made P fertiliser (1.2%) which was 60 times less than a commercial fertiliser.

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OY-07

Immobilization of *Burkholderia cepacia* lipase on eggshell membrane-based carriers

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Introduction

Lipases are versatile biocatalysts that are widely used in the food industry and other areas such as biotechnological and pharmaceutical industry. In their immobilized form, lipases show advantages over free lipases, since it is possible to overcome some of the problems encountered with free lipases use, such as high cost, solubility and reusability in batch and continuous processes. Among different immobilization techniques, adsorption is the simplest method, in which relatively weak interactions are formed between enzyme and carrier enabling the retention of native structure of the enzyme. Since commercial carriers are often very expensive, various waste and/or by-products from the agri-food industry have been increasingly used, among which eggshell membranes are much less studied. Therefore, the aim of this study was to prepare carriers based on eggshell membranes by dissolving eggshell waste with three different acids (5% hydrochloric acid, 10% acetic acid, 15% *o*-phosphoric acid) and to immobilize lipase from *Burkholderia cepacia* by adsorption on the obtained eggshell membrane carriers. The immobilized lipases were tested for their biochemical and operational properties (pH and temperature optimum, pH and temperature stability, stability in organic solvents, storage stability, kinetic parameters, substrate specificity) in comparison with free lipase. The obtained results showed a shift of pH and temperature optimums for immobilized lipases, better temperature stability at high temperatures, and greater storage stability in comparison to free lipase. Additionally, *Burkholderia cepacia* lipase immobilized on eggshell membrane-based carriers of the test biochemical and operational properties was tested on biodiesel synthesis. The results showed that obtained biodiesel met the conditions prescribed by the European standard, i.e. obtained ≥96.5% pf FAME (Fatty Acid Methyl Esters).

OY-08

Can a laboratory predict the field?

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Introduction

Badlands are areas exposed to a wide range of geomorphological processes, scarce or completely absent vegetation formed in a wide range of lithologies in different climate regions. Although great emphasis is placed on the climatic conditions, the complex mineralogical composition and physico-chemical properties of sediments are crucial for badlands formation. Due to that, badland material is suitable for numerous analysis and experiments that provide insight of changes that occur in the field and often attract researchers' attention with the aim to link material properties, weathering and erosion processes which requires understanding both of laboratory analysis and field processes.

In this two-phase study, samples from humid badlands in China and Spain were treated. Four badland samples from each location organised in six sets were treated with rain and acid rain of different intensity and dried at different temperatures. Additionally, three samples from China were organised in four sets and treated also with snow and with acid snow. All of the samples were treated during fifteen daily cycles. Leachate was collected and analysed for monitoring changes in its volume, pH, electrical conductivity (EC) and cation concentration. After each cycle samples were photographed, for physical changes to be tracked.

In rain and acid rain treatment changes in observed parameters were subtle. The Principal Component Analyses implied that during rain cycles sediment decay was caused by physical, and in acid rain treatments by chemical changes. Observing the surfaces of treated samples, it was noticed that high drying temperature presents the most important destructive agent. In normal/acid rain and snow treatments only slight oscillations in measured parameters exist. Physical changes did not indicate drastic differences compared to the sample's surfaces. General differences in observed parameters are noticed more between rain and snow treatments than between their type (normal or acid). The most noticeable change occurred in the measured EC values that are higher in snow than in rain treatments. For better understanding, a ternary diagram was conducted using pH, EC and sum of anions as parameters implying the existing difference between, not only snow and rain treatments, but between normal and acid treatments.

Results achieved in this study contribute to better understanding of behaviour of the treated sediments and the areas that were taken with similar climate conditions and present one step closer to determination of critical properties of material for development of badlands, their further management, as well as to additional classification of dispersive materials.

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OY-09

Evaluating sustainability of direct aptamer assays for the nucleocapsid protein of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2)

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Introduction

Bioanalytical techniques rely on the use of biomolecules, such as antibodies or aptamers, to carry out the determination of the analyte to which they are specific. Though different assays formats have been proposed in the literature, direct assays are especially advantageous in terms of simplicity and sample throughput. In this type of assay, the analyte is immobilized on a solid support. Subsequently, a biomolecule (i.e., tracer), either an antibody or aptamer specific to the analyte, is employed to detect the analyte that has been immobilized. In general, tracer species are conjugated to an enzyme which produces a colorimetric reaction that can be analysed by ultraviolet-visible spectroscopy. Bioanalytical techniques are generally considered sustainable due to their low energy consumption, use of microvolumes, and high sample throughput. [1,2] Nevertheless, there is a potential for further improvement since experimental procedures make use of harmful reagents (e.g., H_2SO_4 for stopping colorimetric reaction) and solid supports are discarded after a single use.

The aim of this project is to assess the sustainability of current aptamer assay procedures, with particular focus on the environmental impact of reagents and the reusability of plates. The nucleocapsid protein of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) is employed as a model analyte in a direct assay to evaluate these aspects. In order to improve the sustainability of the colorimetric detection process, direct absorbance measurement at a prefixed time without stopping the enzymatic reaction was performed and there was not significative difference in the analytical figures of merit. Moreover, it was investigated how to improve support reusability, and it was achieved by employing guanidinium hydrochloride at a concentration of 1 mol L^{-1} for three cycles of one hour each at a temperature of 80 ºC. This resulted in the solid support being reusable up to 5 times without any significative different on the analytical figures of merit. Following these improvements of the sustainability of the direct aptamer assays, the sustainability of the proposed method was evaluated against the reference method (i.e., employing H_2SO_4 1 mol L^{-1} and discarding the plate after each use) employing different metric tools described in literature (e.g., National Environmental Methods Index, the Analytical Eco-Scale, Green Analytical Procedure Index, Analytical GREEnnes, RGB and Hexagon). The results obtained by comparing the sustainability of the methods are not representative of the experimental improvements achieved, as there is no significant difference between the methods. These results can be explained by the fact that the majority of these analytical metric tools do not consider the plastic residues generated by the method and penalise all chemical residues equally, which can lead to inconsistencies in some cases, such as plastic reusability.

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OY-10

Structural features and health effects of water-soluble organic matter from atmospheric fine air particulates

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Introduction

Fine atmospheric particulate matter ($PM_{2.5}$ < 2.5 μm) exposure has been recognized as a key public health issue [1]. Furthermore, exposure to atmospheric aerosols has been associated with higher risks of lung cancer, cardiovascular, and respiratory diseases. PM exposure can also impact the immune system, causing increased susceptibility to infections and pathogens, or aggravating other pre-existent lung diseases [2]. The main mechanisms through which $PM_{2.5}$ can affect the human health, include the modulation of reactive oxygen species (ROS), the triggering or exacerbation of an inflammatory response, and PM-related direct cytotoxicity [3,4]. These toxicological effects have been linked with $PM_{2.5}$ atmospheric concentrations, and its composition in metals and solvent-extractable organics [5,6]. Despite not receiving extensive focus, the ubiquitous water-soluble organic matter (WSOM) present in $PM_{2.5}$ has also been linked with these adverse effects [4]. Hence, it is important to better understand the impacts of this $PM_{2.5}$ fraction.
In this work, the structural features of daytime and nighttime $PM_{2.5}$ WSOM samples from an urban and a rural location will be discussed by means of NMR spectroscopy. Furthermore, a brief overview of the health effects on a human monocytic cell line (THP-1) will be addressed. Some compositional differences were observed between the WSOM samples from the two studied locations. For instance, when comparing the percentage distribution of ^{1}H functional groups of the WSOM samples collected during the cold season, the rural daytime sample was characterized by increased percentages of aromatic and aliphatic saturated moieties, when compared to its urban sample counterpart. Furthermore, regarding the inner-daily variations during this period, the relative distribution of each of the ^{1}H moieties follow an opposite trend when comparing the two sampling locations. Regarding the biological effects on human monocytes, we observed that exposure to the WSOM samples collected during the October period at the urban site led to an increase in the expression of IL-6, IL-8 and TNF-α. Additionally, exposure to these WSOM samples also led to a marked increase in the expression of the HMOX, an important antioxidant gene. Overall, these results suggest that these aerosol WSOM samples are capable to induce a pro-inflammatory state on THP-1 cells.

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OY-11

Sustainable and environmentally friendly processes to synthesise highly stable N-doped activated carbons

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Introduction

The development of electric double-layer capacitors (EDLC) with improved energy density presents important challenges. The lifespan of the EDLC is mainly determined by the stability of the electrolyte. However, the stability of the electrode material is also important for high-voltage charging [1]. Therefore, it is necessary to implement methodologies for the synthesis of materials with high stability for their use as electrodes for supercapacitors, and with lower costs and higher sustainability. Regarding costs, it is important to modify the actual stabilization processes, which usually increase the cost of these materials and have high environmental impacts and develop other methods at softer conditions, like N functionalization of as-prepared carbon materials [1,2]. The environmental impacts of the different stages of a process to obtain nitrogen-functionalized activated carbons using biomass residues as a precursor were studied in a previous study applying the LCA methodology [3]. This study revealed that the main sources of environmental impacts along the process chain come from the functionalization and washing steps, mainly caused by the use of organic compounds [2]. In this work, we have studied the functionalization of activated carbons prepared from biomass residues with N-functional groups through a water-based methodology that reduces the environmental impacts of the process.

Activated carbon was synthesized using almond shell residues as precursor. This activated carbon was functionalized by an organic reaction under mild conditions to introduce nitrogen functional groups using NH_4NO_3 as nitrogen source [4]. Modifications of the process were made to avoid the use of pyridine and ethanol and minimize the environmental impacts generated in the preparation of these activated carbons. Also, the functionalization of a commercial activated carbon was studied using different nitrogen precursors. The activated carbons were used as electrodes of EDLC in organic electrolyte. The stability of the supercapacitors was evaluated by 10000 galvanostatic charge-discharge cycles.

The as-prepared activated carbon has a high BET surface area (>1800 m^2g^{-1}). After the functionalization reaction in water based conditions, nitrogen contents range from ~1.0% to ~3.0%, depending on the carbon material and chemical route used. The incorporation of N occurs in different functional groups and the porosity of the activated carbons was not modified significantly. The functionalized activated carbons exhibited good electrochemical behavior as supercapacitor electrodes and a higher retention of capacitance. The proposed N-functionalization process of activated carbons is very interesting because it avoids the use of organic compounds, allowing to reduce the environmental impacts generated in the preparation of these materials. It is important to highlight that the synthesis methodology used in this work allows the conversion of biomass residues into carbon materials with great potential for use as electrodes in supercapacitors and using a process with reduced environmental impacts.

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OY-12

Bioremediation of industrial brines using *Haloferax mediterranei* R4: the specific case of wastewater coming from a desalination plant, a textile industry, and an olive production company

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Introduction

Haloferax mediterranei has demonstrated considerable potential as a bioremediation agent for brines contaminated with nitrates and nitrites [1], oxychlorides, and certain metals such as Cu [2] and Cd [3]. This suggests its significant potential for bioremediation of salty wastewater [3]. The objective of this study is to assess the capacity of this haloarchaeon to grow and bioremediate industrial waters and brines sourced from a desalination plant (DPR), a textile industry (TIR), and an olive production plant (OPR). Initially, a physicochemical characterisation of these waters was carried out. To compare and evaluate the results, two reference media were employed: an "optimal" medium and a "control" medium, differing in their nitrogen sources (NH_4^+ and NO_3^-) and salt concentrations (20% w/v and 15% w/v, respectively). The industrial wastes exhibited considerable physicochemical heterogeneity; thus, they were not suitable *per se* for the direct growth of *H. mediterranei*. Consequently, they were supplemented with carbon, nitrogen, phosphorus, and iron. Except for the OPR waste, the results indicate that the studied industrial wastes sustain the growth of the microorganism. However, a decline in the physiological response was observed, evidenced by reduced growth rates and lower maximum optical density values. Remarkably, there was an increase in cellular pellet pigmentation, linked to carotenoid production, suggesting elevated cellular stress compared to the optimal and control media [4]. Elemental profile variations showed increases in Fe and Zn values, which are cofactors for metalloproteins associated with stress tolerance [5], and in Ca, which is related to exopolysaccharide production [6]. Despite the observed stress, *H. mediterranei* effectively removed 60-90% of the NO_3^- present in the wastes (used as nitrogen source for cellular growth). These findings suggest that wastewater can be used for the growth of *H. mediterranei*, thus providing a bioremediation approach to valorize waste products and to produce economically and industrially valuable biomolecules.

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OY-13

Detection of persistent, mobile and toxic contaminants in aqueous matrices by high performance liquid chromatography and mass spectrometry

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Introduction

Persistent, mobile and toxic substances (PMTs) represent a significant concern within the context of the water cycle, due to the inherent properties of these compounds [1]. This category of compounds has attracted the attention of European authorities, who have determined that they have a similar level of concern as the persistent, bioaccumulative and toxic (PBT) chemicals that are subject to regulation under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation. The NePMTune project (www.nepmtune.webnode.es) has the objective of identifying and studying the behaviour of PMTs in matrices such as water and urban dust, as well as proposing strategies for their mitigation. As part of the project activities, a suspect screening strategy was developed for the analysis of the presence and origins of PMTs in various aqueous matrices, including river water, raw and treated wastewater, urban runoff, and landfill leachate. A database of 1,100 chemical compounds was constructed for the purpose of suspect identification, employing a prioritisation strategy based on the PBT criteria [2].

In total, 47 samples of the aforementioned types, collected in 2023 across various regions of Spain (Catalonia, Valencian Community and Galicia), were subjected to analysis. Following freeze-drying as a pre-concentration step, screening was conducted using mixed-mode liquid chromatography coupled to high-performance mass spectrometry (MMLC-HRMS), with ion mobility determination (IM-HRMS) as a supplementary technique. A total of 98 PMTs were identified, distributed across the three confirmation levels proposed in the literature [3], with 53 at level 1, 30 at level 2, and 15 at level 3. Furthermore, of the PMTs identified at levels 2 and 3 in the samples, 29 were confirmed with an additional level of confidence using the collision cross section (CCS) obtained by IM-HRMS.

The most frequently identified compounds (representing over 70% of the total) were p-cumenesulfonic acid and 1,3-di-o-tolylguanidine, along with the drugs N-desmethylvenlafaxine, tapentadol and tramadol. Quantitative methods are currently being developed for the most prevalent compounds.

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OY-14

Electrochemical determination of acetylcholinesterase activity for evaluating ecotoxicological threats in marine environments

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Introduction

The presence of pesticides, including herbicides, fungicides, and insecticides residues in food, water, and soil has become a significant issue in the field of environmental chemistry [1]. Organophosphorus and carbamate insecticides are particularly concerning due to their toxicity. Such insecticides inhibit acetylcholinesterase (AChE, EC 3.1.1.7) activity, which is necessary for the proper functioning of the central nervous system of both humans and insects.

Analysis of pesticides in seawater samples is a difficult task due to the matrix complexity and low concentrations of the target compounds. Biosensing methods might overcome the drawbacks of the methods available for the determination of pesticides, like colorimetry [2], capillary electrophoresis (CE) [3] or high-performance liquid chromatography (HPLC) [4]. The mentioned methods have produced successful outcomes, but they have limitations such as difficult and time-consuming sample preparation and can only be utilized in specialized laboratories with costly equipment and trained staff.

Biosensing methods provide advantages such as simplicity, rapidity, specificity, sensitivity, low cost, relatively economical equipment, and user-friendly operation. In this work, we aim at developing an electrochemical biosensor for indirect monitoring of acetylcholinesterase to detect pollutants such as carbendazim or malathion in seawater.

AChE has a very high catalytic activity; each molecule of AChE degrades approximately 25,000 molecules of acetylcholine (ACh) per second into choline and acetic acid. AChE belongs to the family of hydrolases and its active site is characterized by a catalytic coordinated triad of three essential amino acids. However, in the presence of an inhibitor such as carbamates or organophosphorus, a blocking of the triad occurs, and the enzyme is inactivated. Keeping in mind the above mentioned, the catalytic activity of the enzyme has been studied by cyclic voltammetry, using p-acetoxyphenol as a substrate, which lacks of electrochemical response. As a result of the hydrolysis, an electroactive product (hydroquinone) is obtained, which can be electrochemically detected.

The most important step in the development of an enzyme-based electrochemical sensor is that the enzyme must stay fixed. For that, the enzyme is encapsulated in a sol-gel silica matrix. Through kinetic studies, the activity in the hydrolysis reaction of p-acetoxyphenol was checked. After that, inhibition studies were conducted in the presence of malathion at various concentrations. The results revealed a relationship between the inhibition of enzyme activity and the concentration of added pollutants. This system may pave the way to be utilized in the design of a biosensor-based device that can detect contaminants in the marine environment at an early stage.

Acknowledgements

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OY-15

Optimizing the recovery of Rare Earth Elements from aqueous mediums using easily separated manganese ferrites

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Introduction

The successful implementation of the UN's sustainable development goals heavily depends on the sustainable management of natural resources. The rare Earth Elements (REE) have been increasingly used in many hi-tech applications such as hybrid vehicles and renewable energy technologies. However, these elements are obtained unsustainably from primary mining activities within a restricted number of countries (mainly China) which cause severe negative impacts on the environment. Potential disruptions in the supply chain of the REE have fuelled the search for innovative and sustainable technologies to recover them from alternative sources [1]. Although solvent extraction is the most widely used technique, adsorption technologies have also emerged as a simple, cost-effective and environmentally benign choice to recover these elements from aqueous solutions [2]. Despite these benefits, one of the main drawbacks of adsorption technologies is the lack of an efficient way to recover the adsorbents from the solution, often requiring energy-intensive processes such as filtration or centrifugation for their retrieval. In this context, the use of magnetic materials which can be easily separated from a solution through the application of an external magnetic field seem like an easy way to circumvent this issue. Because of this, and due to previously established high sorption capacity [3], magnetic manganese ferrite nanoparticles ($MnFe_2O_4$) are a promising material to be used in REE recovery.

In this study we applied $MnFe_2O_4$ nanoparticles to a solution spiked with 9 REE (Y, La, Ce, Pr, Nd, Eu, Gd, Tb and Dy) and optimized the sorption conditions for of pH (4-8), mass of material (20-180 mg/L) and concentration of REE (1-5 µM for each REE) using surface response methodology. Additionally, we studied the adsorption kinetics as well as the effect of increased salinity (0-30 mg/L of NaCl).

Our results indicated that high pH favoured REEs sorption because of the material's surface charge, which promoted interactions with REEs ions at pH 6-8. At lower pH, the surface of the material becomes positive, repelling the positively charges REE species, and thus decreasing sorption. For the lowest concentration of 1 µM, 100 % removal for all elements was achieved with 151 mg/L of material at pH 8. For the highest concentration of 5 µM, all elements (except Y) were totally removed using approximately 170 mg/L of material at pH 8. Sorption efficiency for Y was consistently lower than that of the remaining elements. Salinity did not impair sorption significantly (< 10 %), which was owed to the high sorbent mass used in those assays. An increase in sorbent mass and initial REEs concentration also promoted faster kinetics. Multiple adsorption cycles were performed, and the material did not display a decrease in sorption efficiency even after 5 cycles, highlighting its reusability. Desorption of REE from the nanoparticles was easily achieved within 30 min using HNO_3 0.1 M. The spinel type $MnFe_2O_4$ nanoparticles showed great promise in the recovery of REE from complex solutions and represent an optimistic prospect for a realistic application, which is the next proposed step in this line of research.

Acknowledgements

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OY-16

Portable cost-effective colorimetric detection of polycyclic aromatic hydrocarbons using an iPhone 11 camera

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Introduction

Polycyclic aromatic hydrocarbons (PAHs) are a prominent diffuse pollutant in urban waters due to runoff from natural weather events. Their source is mainly anthropogenic activity, specifically the incomplete combustion of fossil fuels for motor vehicle propulsion and domestic heating. The expulsion of these pollutants into the atmosphere ultimately results in their presence in urban waters. As of 2024 the adopted standard by the European Union is that drinking water must have no more than 0.1 µg/L bulk concentration of PAHs and 0.01 µg/L of benzo[a]pyrene, one of the most carcinogenic and infamous species.[1] Current analytical methods for detection of these compounds are mainly GC-MS and HPLC with UV or fluorescence for detection, which can require significant solvent consumption, labour and time. Novel developments in analytical instrumentation aim for the development of on-site testing devices with the use of microfluidic technology reducing solvent and sample volume while also making devices smaller, cheaper, and portable.[2]

This work presents a colorimetric assay for detection of a range of PAHs using citrate stabilised 15 nm gold nanoparticles. In the presence of PAHs, the gold nanoparticles aggregated causing a red to purple colour change, which allowed for their quantitative detection by UV-vis spectrophotometry. Furthermore, the use of a smartphone camera allowed for on-site analysis in a microfluidic chip. Pictures taken with an iPhone11 camera were processed using the ImageJ software to generate a calibration for the analyte. Ultimately, the integration of smartphone detection in combination with the advantages of lab-on-chip (LOC) microfluidics will provide a cheap, robust, and rapid quantitative tool for on-site monitoring of PAHs in urban water runoff samples.

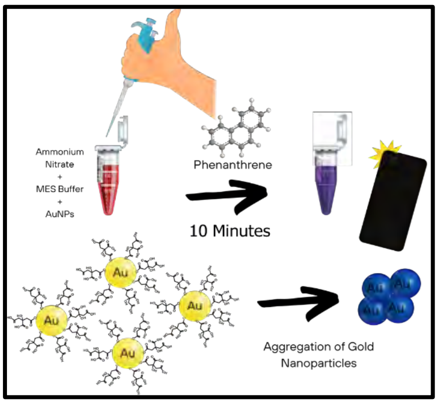

Figure 1 – PAH induced aggregation of colloidal gold

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OY-17

Study of PFAS contamination in drinking waters of the Fos-Berre area (France)

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Introduction

Per- and poly-fluoroalkyl substances (PFAS) are composed of thousands of substances whose unique physicochemical properties such as water and grease repellence, non-sticking and heat resistance [1] have made them essential in many industrial fields like firefighting foams, electronics, food contact materials and the textile industry [2]. However, they are released during production and use into every environmental compartment [3], leading to an exposition and impregnation of all organisms. The monitoring of PFAS in environmental and biological matrices is highly needed owing to their bioaccumulative [4], persistence and toxic [5] behavior. For that purpose, the analytical technic should be very sensitive to achieve detection at ultra-trace levels (ng.L^{-1}).

An analytical method has been developed to investigate 35 PFAS in tap water, belonging to either the ISO 21675 standard or the Classified Installations for the Protection of Environment (PCI) regulation and including the 20 PFAS regulated by the 2020/2184 Water Framework Directive (WFD). Tap water samples have been collected in a highly industrialized area in the South of France to establish both contamination levels and geographical distribution of the quantified compounds. Water samples were collected in 28 sites in high-density polyethylene (HDPE) bottles, pre-washed with ultra-pure water, methanol and three times with water from the sampling site. Field blanks were made by filling HDPE bottles with ultrapure water on site and exposing them to the sampling environment, to investigate the contamination risk during sampling and sample transport. Ammonium acetate was added as a preservation agent. Samples were transported in a cooler at a temperature around 4°C and stored frozen until analysis through injection on LC-MS/MS, within 2 weeks after collection. Solvent blanks were run before and regularly within each batch to perform analytical blanks and investigate the instrumental background as well as potential carryover contamination. The precision and accuracy of the method were confirmed for each run and monitored by the regular analysis of calibration points. Method accuracy has been evaluated through the analysis of a CRM and by having duplicated samples analysed by a certified laboratory. Over the 35 PFAS investigated, 12 were quantified in at least 1 sample. Despite the taken precautions, some contamination was found in the field blanks and was therefore subtracted from the sample signal when relevant (blank percentage below 25%). The sum of total PFAS was below the 2020/2184 WDF limit for all samples, and the sum of the 20 regulated PFAS was above the limit for only 1 sample. The difference in contamination levels and profiles over the 28 sites indicate an influence of the nearby industries.

Acknowledgements

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OY-18

Understanding the degradation of bio-based polymers across contrasting marine environments

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Introduction

Biodegradable and compostable polymers have emerged in recent decades as an alternative to conventional plastics to mitigate environmental problems related to plastic pollution. This study examined the degradation of bio-based materials certified as biodegradable or compostable through a laboratory experiment for one year. The materials were exposed to three compartments of the marine environment, including the seabed and both the euphotic and aphotic zones of the water column. The degradation rates and pathways of bio-based materials were evaluated combining weight loss, Fourier-transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) before, during and at the end of the experiment. The degradation rate of the studied bio-based polymers was highly influenced by the environmental compartment, being degraded *ca.* 5 times faster in the sediment than in the water column. However, light did not play a key role in the weight loss of the materials submerged in the water column. Our results showed that the simultaneous use of the parameters derived from the three analyzed analytical techniques, specifically the FTIR derived indices, the maximum degradation temperature, the activation energy and the melting enthalpy, gives a complete understanding of the degradation process of a specific biodegradable/compostable polymer in different environmental compartments. Having a deeper understanding of the biodegradation mechanisms of bio-based materials is essential to develop more sustainable materials. Our findings emphasize the need to go one step further to develop new technical standards that certify the degradability of the materials embracing different environmental compartments.

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OY-19

Emerging organic contaminants degradation and faecal bacteria indicators elimination by a new filterless domestic purification system

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Introduction

Many emerging organic contaminants (EOC) are found in waters, including drinking water resources [1]. The occurrence of pharmaceuticals, pesticides, PFAS, hormones, surfactants, and transformation products in tap and drinking water has been assessed at trace level of 1 ng.L^{-1} to 10 µg.L^{-1} [1]. Although these contaminants do not seem to represent individually a health hazard at this level [2], the impact of a long-term exposition to EOC is still uncertain [3]. Moreover, inefficient disinfection and/or micro-organism development in plumbing can induce the presence of opportunistic pathogens, representing an emerging water borne disease problem [4]. To overcome these dual public health issues, new domestic water purification systems (DWPS) have been developed. LaVie is a new DWPS, developed by Solable society (France), based on an advanced oxidation process (AOP), combining the residual free chlorine (FC) present in tap water and a LED-UV A irradiation source. Studies focusing on the degradation capacity of LED-UV A / FC AOP in drinking or tap water matrices are still very scarce, as it represents an important research prospect to assess the purification capacities of emerging and domestic AOP systems and gain a better understanding of their potential applications.

EOC degradation and disinfection capacities of LaVie system in tap water has been investigated through a general kinetical study. Atrazine, bisphenol A, carbamazepine, clofibric acid, N,N-Diethyl-meta-toluamide, desethyl atrazine, 17-α-ethynylestradiol, ibuprofen and metolachlor have been selected for their recurrence in tap water resources [1]. The degradation of these 9 EOC has been followed at relatively high concentrations (1 to 5 mg.L^{-1}) in the presence of different amounts of free chlorine (0 to 3 mg.L^{-1}) to be representative of world tap water content. Degradation rates revealed to be in the range 2 to 95%, depending on the EOC, free chlorine concentration and exposure time. For the disinfection capacity assessment, the elimination of 2 *Escherichia coli* strains (ATCC 15 597 and 11 303) and 2 *Enterococcus faecalis* strains (ATCC 19 433 and 33 186) as well as their revivification capacity after 24h were explored at high concentrations (10^3 to 10^4 CFU.L^{-1}) in representative experimental conditions (free chlorine from 0 to 0.2 mg.L^{-1}). Disinfection efficiency varied from 0 to 99% depending mostly on the bacterial strain. No revivification capacity has been observed.

Acknowledgements

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OY-20

Energy-efficient UASB de-ammonification for wastewater management

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Introduction

This study explores the integration of anaerobic treatment and deammonification technologies in wastewater management, focusing on their application in both lab-scale and pilot-scale systems. The research aims to evaluate the effectiveness of these combined processes in enhancing the removal of key pollutants from domestic wastewater. In the lab-scale phase of this study, the research focused on optimizing the anammox process within a controlled environment to establish the most effective conditions for organic and nitrogen removal from domestic wastewater. The lab-scale experiments were essential in fine-tuning the operational parameters, such as the nitrite-to-ammonium ratio and hydraulic retention time (HRT), to maximize the efficiency of the anammox bacteria in the Moving Bed Biofilm Reactor (MBBR) system. By simulating different scenarios, the lab-scale study provided critical insights into the microbial dynamics and pollutant removal efficiencies under various conditions, laying the groundwork for scaling up the technology. Following the lab-scale optimization, the pilot plant was constructed with a capacity of 100 KLD to validate the findings on a larger scale and in real-world conditions. This pilot plant combined anaerobic treatment with deammonification, leveraging the optimized anammox process identified in the lab. Over a six-month operational period, the pilot plant demonstrated significant improvements in removing pollutants, achieving removal efficiencies of 93% for COD, 94% for TSS, 95% for total nitrogen, and 91% for total phosphorus. These results confirmed that the integration of anaerobic treatment and deammonification in the pilot-scale plant was not only feasible but also highly effective, consistently producing effluent that met the required standards for discharge or reuse. The comparative analysis between the lab-scale and pilot-scale operations highlighted the scalability of the anammox-MBBR system, showcasing its potential for broader application in domestic wastewater treatment. This transition from lab to pilot scale provided valuable insights into the challenges and successes of implementing advanced treatment technologies in a practical, real-world setting.

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OY-21

Enhancing microbial electrosynthesis with polyaniline as cathode catalyst for CO_2 capture and conversion to green chemicals

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Introduction

Microbial electrosynthesis (MES) is a method that effectively converts CO_2 into valuable chemicals, mainly acetate, using minimal energy. Nonetheless, the low product concentration has constrained its large-scale application. This challenge can be mitigated by employing biocompatible cathode catalysts. Designing catalysts with a high surface area and high electrical conductivity has proven to enhance biofilm formation, improve CO2 reduction, and boost hydrogen evolution reactions. Optimizing the electrode surface interface plays a crucial role in facilitating electron uptake by electroactive microorganisms thereby promoting efficient extracellular electron transfer systems. This process is crucial for increasing the synthesis of acetate from CO2. Polyaniline (PANI) is a highly conductive polymer that has great potential for use in electrode development. This is because PANI possesses excellent biocompatibility, and thermal stability, and is cost-effective. Carbon felt (CF) is commonly employed as a conductive material in the fabrication of composites due to its stable physicochemical properties, favourable cost-effectiveness, and convenient availability. It is an exceptional material for creating devices of various forms and promoting biofilm growth. For this study, composite electrodes were developed through the In-situ chemical oxidative polymerization of aniline in the presence of a carbon felt. The efficacy of the PANI-coated CF electrode was assessed by comparing the rate of synthesis of organic compounds and electrochemical properties. The electrochemical properties of the electrode have been explored through the utilization of cyclic voltammetry and electrochemical impedance spectroscopy. The physicochemical properties of the electrode were analysed by X-ray diffraction (XRD), Scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM-EDS), and Fourier transform infrared spectrometry (FTIR). The use of PANI as a cathode catalyst led to a significant 2.36-fold increase in the maximum concentration of acetate, reaching an impressive 8.823 g L-1 compared to the MES run without a cathode catalyst. The carbon felt electrode, modified with PANI, demonstrated improved microbial adherence and greater electron transfer between the electrode surface and microbes. These enhancements were significant in enhancing the performance of the MES. Therefore, PANI may be regarded as a very effective cathode catalyst in MES to increase the acetate yield rate.

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OY-22

Investigation of sorption and photochemical capacity of sewage sludge derived biochar for the removal of water contaminants

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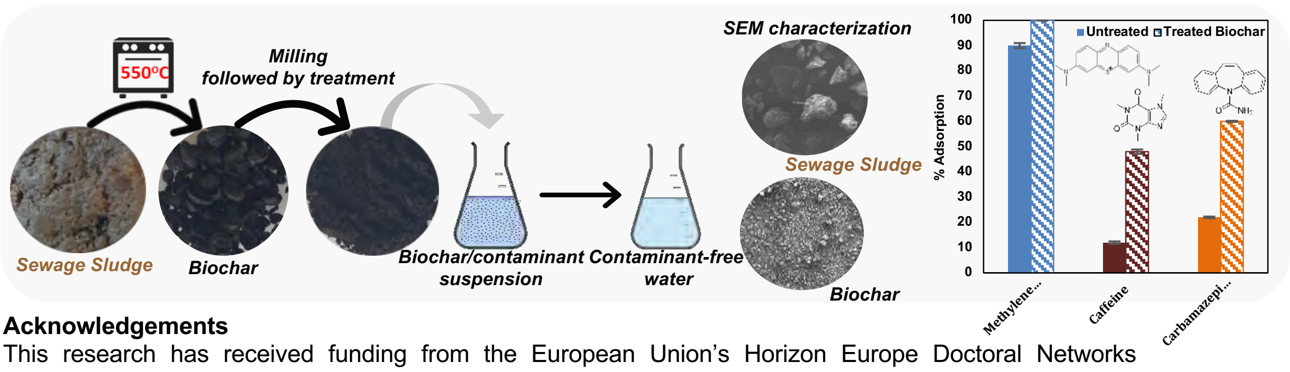
Introduction

Annually, millions of tons of sewage sludge (SS) are generated during wastewater treatment. In 2022, over 4 million tons of SS on a dry weight basis were produced by European Union member states [1], with disposal and processing expenses accounting for nearly 50% of the total operational costs of wastewater treatment plants [2]. Currently, common disposal methods include incineration, landfilling, and agricultural reuse [3]. An emerging and promising alternative is the thermochemical conversion of SS into biochar, an activated carbon-like material. Biochar has the potential to remove pollutants from wastewater effluents, thereby advancing the circular economy by converting waste into a valuable resource.

This research, conducted in the framework of the European project IN2AQUAS, focuses on developing sustainable materials for water decontamination. The study investigates materials derived from SS and biochar for contaminant removal via sorption and photochemical processes. Sewage sludge and biochar pyrolyzed at 550°C were mechanically milled, activated, and characterized. The biochar samples had an average particle size of 8 μm, a surface area of 43 m²/g, high carbon and oxygen content, and contained small levels of iron.

Three organic pollutants—methylene blue, caffeine, and carbamazepine—were selected for evaluation. Experiments involved adding biochar particles to water containing these contaminants. Results showed effective removal of methylene blue, with an initial concentration of 10 mg/L and non-activated biochar at 1 g/L. In contrast, removal of caffeine and carbamazepine under the same conditions was below 25%. Activated biochar demonstrated enhanced performance, increasing carbamazepine adsorption by 40%. The mechanisms underlying these observations are currently under investigation. Kinetic and adsorption equilibrium studies were also performed, with different models having the best fitting over the experimental results, depending on the contaminant.

Under irradiation, SS was also found to produce reactive oxygen species (ROS) indicating its potential use in photochemical water treatment processes. Research is underway to explore the efficiency of biochar and SS-derived photoactive composites incorporated into water filtration membranes, for effective, sustainable, and cost-efficient contaminant removal.



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OY-23

Study and modelization of an electrodialysis process for saline wastewater regeneration and reuse in agriculture

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Introduction

Water is a scarce resource along Spain's eastern Mediterranean coast. Due to the proximity to the sea and the deficiencies in the local pipeline infrastructure, seawater intrusions occur into the wastewater system. Saline wastewater pose a challenge for wastewater treatment plants (WWTPs), as it hinders water reuse and sustainable discharge. At Santa Pola WWTP (Latitude: 38.219109; Longitude: -0.562122) these intrusions result in conductivities between 4 to 5 mS/cm, primarily due to the presence of the salts such as NaCl and Na_2SO_4. However, current regulations require conductivities below 3 mS/cm for water reuse in agriculture or safe discharge into natural channels. To approach this issue a tertiary treatment system is proposed, and consists of two processes:

1. Electrodialysis (ED) system, a membrane process of separation under the action of an electric field, where ions are selectively transported across specific membranes. Properties such as selectivity, ion-removal efficiency, and chemical-free treatment make ED process adequate for partial desalination of brackish wastewater with significant environmental benefits.

2. Electrochlorination (EC) system that will use the brine produced by the ED. In order to reduce the conductivity of regenerated water to, at least, 3 mS/cm, and exploit the residual concentrated brine to produce sodium hypochlorite (NaClO), a disinfectant currently used in the WWTPs.

Both processes are being investigated initially at laboratory scale, with this study focused on the ED system.

The ED reactor, provided by EURODIA Industries, has been characterized under ion concentrations and conductivities based on the real compositions of the treated wastewater from the Santa Pola WWTP (data obtained by analysis of the real waters from different years and seasons). With the results, a mathematical model has been developed to predict the reactor's behavior not only at lab-scale, but also at pilot scale, a critical step for scaling up the process to the implementation at the WWTP. Some of the parameters analysed in the model are the resistance of the components (membrane, solution, among others), the mass transfer coefficient (km), the volume variation in the tanks, the temperature, etc.

Once an initial approach to the system has been taken using synthetic water, real brackish wastewater will be used to check the obtained values and to assess the effect of additional factors like the impact of organic matter contamination has in the reactor behaviour. These insights will later be incorporated into the mathematical model to ensure accuracy. The results of this research will allow to successful implementation and study of the integrated ED-EC system at the Santa Pola WWTP in the immediate future, contributing to more sustainable water management in the region.

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OY-24

Titanium dioxide – Carbon Dots nanocomposites for the visible-light and sunlight-driven photodegradation of organic pollutants

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Introduction

Water is arguably the most crucial resource on Earth. The efficient removal of pollutants such as dyes and pharmaceuticals, which are deemed persistent organic pollutants, is essential to preserve our water resources, something which conventional wastewater treatments are not capable of. [1] As an alternative, photocatalytic technologies may achieve a near-complete degradation of the pollutants by harnessing the energy of a light source, such as solar irradiation. Titanium dioxide (TiO_2) is a stable and inexpensive photocatalyst that is widely used across several areas, [1] despite presenting some limitations: requiring high-energy UV radiation, which is only a small fraction of solar radiation; suffering from rapid charge recombination, lowering its photonic efficiency; and poor affinity towards organic compounds. [2]

Combining TiO_2 with carbon dots (CDs) may be a solution to bridge these limitations. [2] CDs are carbon-based nanoparticles with interesting properties, such as high photoluminescence, broadband absorption, and good water solubility. Their interesting properties and the easiness of their preparation enable the use of CDs for several applications, including sensing, LEDs, and photocatalysis, among others. [4]

Herein, we report the conjugation of CDs with TiO2 to form efficient photocatalytic nanocomposites for the visible-light-driven photodegradation of organic pollutants. In the first stage, by adding CDs, we developed a composite with an enhanced potential for the photodegradation of methylene blue (MB), increasing the efficiency by 367% compared to bare TiO_2 (Figure 1). [5] Via Life Cycle Assessment studies, we observed that, when considering the function for which they are intended, the nanocomposites have a lower relative environmental impact than bare TiO_2. Building on this, we modified the composite to include some waste materials as part of the CDs, thus promoting a circular economy while maintaining performance. Finally, we tackled the removal of ciprofloxacin using this method, achieving a virtually complete degradation of 20 ppm of ciprofloxacin within 20 minutes of sunlight irradiation with the addition of the CDs significantly improving the efficiency when compared to bare TiO_2.

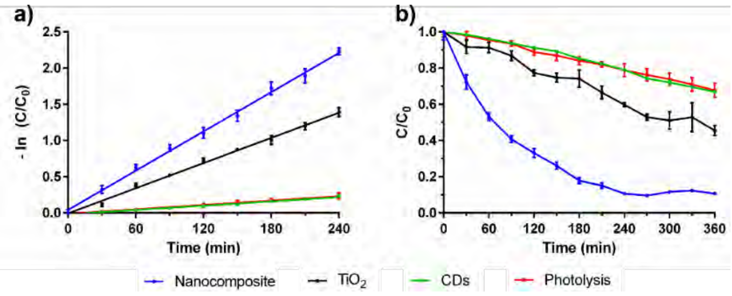

Figure 1 – Representation of the a) reaction rate constant and b) C/C_0 for the photodegradation of MB.

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OY-25

Unravelling UV-induced photochemical mechanisms for nano-polystyrene removal from water

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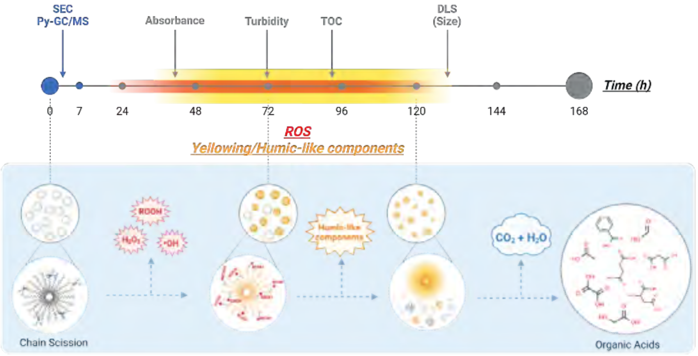
Introduction

During human-induced disposal or natural weathering, plastics undergo fragmentation or degradation into smaller particles, which can be defined as microplastics (MPs, 1 µm to 5 mm) or nanoplastics (NPs, 1 to 1000 nm) depending on their sizes [1]. The small-sized plastic fragments pose a greater threat to ecosystems and humans than larger plastic pieces, which has attracted global concern. In particular, there is limited understanding of the environmental behavior of NPs due to their size, complex physical-chemical properties, and the limitations of current detection technologies. Consequently, it is urgent to develop effective and environmentally sustainable methods for the removal of NPs from aquatic environments.

In this study, we focused on applying different homogenous advanced oxidation processes (AOPs) for the removal of nanoparticles of polystyrene (Nano-PS) from water, evaluating the impact of different UV-induced oxidation processes on the apparent color and turbidity of the suspension, microscopic morphology, dynamic size, molar weight, UV characteristic absorption, and intermediate products. Specifically, the dynamic changes of reactive oxygen species (ROS) such as •OH, H_2O_2, and ROOH during the reaction process were monitored using fluorescence spectrophotometer and high-performance liquid chromatography (HPLC) techniques.

The photoaging of Nano-PS induced by photo-based AOPs is shown in the Fig.1. The UV irradiation could induce Nano-PS to generate ROS, which subsequently attack the surface of Nano-PS, resulting in the production of yellowing discoloration and humic-like components. These products are also precursors of ROS, ultimately contributing to the oxidative degradation of Nano-PS. Additionally, different light sources (UVA, UVB and UVC) could influence the composition and amount of ROS generated, thereby affecting the reaction time scale. Furthermore, the introduction of oxidants (H_2O_2) significantly impacts these photochemical processes, either positively or negatively depending on the light sources.



**Time for removal rate to reach 30%*

Fig.1 Schematic illustration of Nano-PS photoaging behavior in water.

The qualitative and quantitative analysis of Nano-PS in the AOPs and quantitative monitoring of ROS can help us to understand the behavior of Nano-PS in the environment, which also provides a scientific basis for the development of effective nano-pollution control strategies.

Acknowledgements

This work was supported financially by ANR AOPNANOP and Chinese Scholarship Council. The authors thank Guillaume Voyard for his valuable contribution in IC/MS analysis.

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P-AgroEnv-01

From the soil to the wine – elements' migration in monovarietal Bulgarian wines

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Introduction

Bulgarian wines are famous worldwide and are one of the country's symbols. Chemical elements transfer in the system soil/grape/wine is important factor defining wine's quality and authenticity. In the present research a total number of 34 monovariety Bulgarian wines with proofed geographical and botanical origin were analysed for 44 chemical elements (essential, potentially toxic, rare-earth). White wines were presented from Chardonnay, Muscat Ottonel, Sauvignon Blanc, Tamyanka, Viognier. Red wines were produced from Egiodola, Broad Leaved Melnik, Cabernet, Cabernet Franc, Cabernet Sauvignon, Marselan, Melnik, Merlot, Pinot Noir, Syrah.

The chemical elements' contents in the wines are related on the one hand naturally with their levels in soils and hence in the grapes. On the other hand, the anthropogenic influence: fertilizers with which the soil was cultivated, irrigation water and also possible contamination from the vessels during wine storage. The chemical elements content was determined in the soil extracts (acetate and EDTA as potential bio accessible fraction), vine leaves, musts, and final raw wines before any clarifying and stabilizing. From the obtained results the statistically significant correlation coefficients (>0.5) were calculated for the system soil extract acetate/EDTA – leaves – must – wine. The Self-organizing maps technique was used for the optimization of the variables set and for the separation of wines into different clusters according to the botanical origin.

Acknowledgements

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P-AgroEnv-02

Application of hydrolytic enzymes for the removal of fats and oils from wastewater

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Introduction

The unchecked growth of the global population and its increasing demand for resources and food have led to a considerable increase in meat and cooking oil production. This surge has led to a sharp rise in the number of animals, slaughterhouses and meat production in recent decades [1]. The expanding meat and edible oil industry generate large quantities of oily and fatty wastewater which, if not properly treated, pose a significant threat to the environment and aquatic ecosystems due to their high organic and inorganic load. Lipases are the most commonly employed enzymes in the treatment of oily and fatty wastewaters as they can break down fats and oils into simpler free fatty acids (FFA) and glycerol. However, lipases are generally used for the pre-treatment of such wastewaters and must be combined with other treatment methods (e.g. activated sludge) to ensure complete removal. Immobilization of enzymes on a solid support increases their stability, reusability and control over the reaction processes, thus improving their efficiency for industrial applications. In line with the principles of a circular economy, the use of various production residues as carriers offers a sustainable approach. In this study, by-products from the food industry, in particular eggshell membranes, were used as carriers for the immobilization of commercial lipase from *Burkholderia cepacia* [2]. The results showed that immobilized lipases from *Burkholderia cepacia* effectively removed FFA from synthetic wastewater, although further research is needed to optimize the process.

Acknowledgements

This work has been fully supported by Croatian Science Foundation under the project IP-2020-20-6878 (ImoLipWaste).

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P-AgroEnv-03

Thermal processing effect on element absorption from honey bee (*Apis mellifera*) feed

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Introduction

Recently it was shown that micronutrient deficiency in honey bees may be associated with the widespread chalkbrood disease [1], caused by the fungus *Ascosphaera apis.* To address this, we have begun exploring the use of yellow mealworm larvae (*Tenebrio molitor* L.) flour as a potential substitute for pollen in bee diets.

Our current focus is to determine how thermal processing of this food, affects the absorption of essential elements by the bees. Honey bees were divided into two groups consisting of five cages each, with about 100 bees per cage. They were kept in an incubator at 35° C and RH 70%. All 10 cages were supplied with a piece of drawn-out comb, tap water and 35 g of specific patty partially enveloped with plastic wrap to prevent drying. First group of five cages (NT) were supplied with patties with non-autoclaved mealworm flour for 8 days, those patties were than replaced with patties with autoclaved mealworm flour for next 10 days. Second group of five cages (AT) were supplied with patties with non-autoclaved mealworm flour during whole experiment (18 days). After 18 days gut (midgut and rectum) was rapidly removed using tweezers. Element concentrations were done separately from the gut and rest of body.

About 100 mg of freeze-dried and homogenized sample was digested in an ultraCLAVE IV microwave digestion system using 5 mL of concentrated HNO_3. Each digestion was accompanied by three digestion blanks (5 mL conc. HNO_3) and three reference materials BOVM-1 "Bovine muscle powder". Element concentrations were determined using ICPMS. NA group of bees was first kept on non-autoclaved patties for the first 8 days of bee rearing, because soon after emergence young bees start to consume protein rich food (beebread). Afterword it was replace so as to observe whether nutrition in first days of life has a long-term impact honey bee nutrition status and body composition.

Significantly higher concentration of K, B, Rb, Ba, Ag and Pb was detected in bodies of AT group in comparison to NT group of bees. There was no statistically significant difference in other tested elements, except for Fe that was to only element that was higher in NT group in comparison to AT group. Only element that was detected in significantly higher concentration in the gut NT bees was Pb, there were not significant differences between other tested elements. At the same time Pb is lower in NT group. This confirms that Pb is more efficiently absorbed from autoclaved food in comparison to non-autoclaved food.

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P-AgroEnv-04

Optimization of a sensitive methodology based on ultrasound-assisted extraction emulsification microextraction (USAEME) and high-resolution mass spectrometry for the analysis of multi class herbicides in water

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Introduction

Due to the increase of world population, the agricultural sector remains fundamental in order to meet the growing global demand for food, while preserving the environment. Achieving this goal implies the development of sustainable agricultural and farming methods, which includes the use of pesticides that may pose significant health risks (e.g., carcinogenicity, mutagenicity, and reproductive toxicity), environmental hazards (e.g., toxicity to aquatic life with long-lasting effects) and risks for food/feed safety.

Once applied on the field pesticides can be transported and transformed through different physico-chemical process (degradation, transformation, photolysis, sorption-desorption and leaching). One of the main causes of ground and surface water contamination by pesticides is the movement and the fate of the active substances through the soil, which is governed by meteorological conditions, the chemical properties of the compounds and the texture and organic matter contents of the agricultural soils. Besides, the use of organic amendments like biochar (plant material from pyrolysis) can help to prevent and remediate contamination in soil and water.

The present study focuses on the development of a sensitive analytical method for extracting and quantifying herbicides from/in water. The targeted active substances, mainly used in maize crops, feature diverse characteristics and include two low-dose sulfonyurea herbicides (rimsulfuron and nicosulfuron), a biopesticide (spinosad), a highly utilized and rapidly degraded aromatic ketone herbicide (mesotrione), and a chiral imidazoline herbicide (imazamox). The study also includes other “old” herbicides previously applied for several years in plots of maize and winter crops, such as terbuthylazine, metolachlor, prosulfuron and dimethenamid.

To achieve the goals, ultrasound assisted emulsification microextraction (USAEME), which implies the use of a low amount of extraction solvent, was employed and followed by liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS/MS).

Various influential factors such as the pH, salt addition, extraction time, and extraction solvent were investigated and optimized by means of an experimental design. After establishing the optimal extraction conditions, the method was applied to environmental waters.

The first results revealed the high sensitivity and robustness of the USAEME method combined with LC-HRMS/MS, reaching concentrations at the low ng L^{-1} for many of the target analytes. Future studies will focus on the extraction and analysis of the target herbicides in soil cores collected between 10 and 30 cm of depth in experimental maize plots amended with biochar.

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P-AgroEnv-05

Brewers' spent grain and wild edible herbs as starting material for new functional confectionery products

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Introduction

In recent years, science and the food industry have focused specifically on functional foods with particular health benefits. Cereal residues, which make up about 85% of all by-products in the beer industry, represent the main waste of this industry, in which the husk of barley grains is the most abundant. Brewers' spent grain (BSG) is composed of lignocellulosic biomass rich in protein (20-30%), fiber (30-70%), and minerals. This waste has significant nutritional value and is desirable for human consumption. Since the ingredients used in brewing are approved for human consumption, this by-product can be safely used to develop new food products. The potential of BSG has not been significantly exploited for food intended for human consumption, so this study proposes its use as a cheap and nutritionally rich food ingredient in the confectionery industry. Because of their high dietary fiber content, BSG-enriched foods may provide significant health benefits, such as preventing heart disease, cancer, diabetes, and gastrointestinal disorders. Consuming biscuits enriched with BSG would favor the digestive system and reduce the level of lipids and cholesterol in the blood. Adding BSG can enrich the biscuit with fibers, proteins, and minerals, giving it a new, pleasant taste and good sensory properties. This study showed that BSG can be processed into flour and used as a substitute for wheat flour in confectionery products. Wild edible herbs whose ingredients show antimicrobial, antiviral, and anti-inflammatory properties can also be a valuable addition to biscuits. Wild edible herbs contain biologically active phenolic compounds, which show high antioxidant activity and the ability to remove free radicals. In this study, biscuits were made by substituting 10%, 20%, 30%, and 50% of wheat flour with flour obtained from BSG. These different flour mixtures were used to prepare the biscuit dough, which was then baked for 20 minutes at 150°C (Figure 1).

Figure 1. Biscuit samples based on the brewer's spent grain

This paper shows an innovative way to turn "spent" grains into "saved" grains by valorizing by-products into functional biscuits. The biscuits were additionally enriched with several wild edible herbs, improving their functional and sensory properties. A preliminary examination of potential consumers' acceptability showed that the biscuit sample, in which 20% of the wheat flour was replaced by BSG flour, was the most sensory acceptable. Therefore, this wheat flour and BSG flour (80/20) ratio was further used to make biscuit samples, with the addition of wild edible herbs. The water activity (aw) was in the range of 0.53-0.59, which is acceptable for preserving biscuits' microbiological, chemical, and physical stability.

Acknowledgements

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P-AgroEnv-06

Biological effectiveness of newly synthesized [NiL $(H_2O)_2$] on fungy *Phomopsis viticola*

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Introduction

Starting from the practical application of pyrazole derivatives as active substances in fungicides [1] and previous experimental scientific research [2,3], this work initiates activities to determine the biological effectiveness of the newly synthesized [NiL$(H_2O)_2$] complex on the development of the mycelium of the fungus *Phomopsis viticola Sacc*. in laboratory conditions.

For the synthesis of potential fungicidal active substances, a representative selection of metal salts such as Ni(II)acetate and pyrazole ligand 3,4 (chlorophenyl-1Hpyrazole) (L-$C_9H_7ClN_2$) was made. We note that the selected pyrazole ligand was not used in syntheses and biological tests so far, unlike Ni(II)acetate.

The biological effectiveness of the newly synthesized and structurally characterized Ni(II) complex is reflected in the measurement of the diameter of the mycelium of the fungus *Phomopsis viticola Sacc*. (in a set of four measurements) after treatment with the Ni(II) complex compared to the control sample.

The diameters of *Phomopsis viticola* mycelia of prepared Ni(II) complex samples in the range of concentrations ($1\cdot10^{-3}$% $5\cdot10^{-4}$%; $2\cdot10^{-4}$% and $1.25\cdot10^{-4}$%) were processed by analysis of variance, and testing of means values was performed using the LSD test (LSD_{50} (0.01) =0.879). The results of biological effectiveness indicate that the initial concentration of $1\cdot10^{-3}$% (middle) from the applied range of Ni(II) complex showed a fungicidal effect on the fungus *Phomopsis viticola* (reduction of the diameter of the fungus by 1.1cm compared to the control sample). At the same time, the inhibitory effect of the concentrations of $2\cdot10^{-4}$% and $1.25\cdot10^{-4}$% (II and III measurements) of Ni(II) complex samples was determined, which is reflected in the reduction of the diameter of the mycelium of the fungus Phomopsis viticola by 1.5cm and 1.0cm compared to the control sample. (LSD_{50} (0.01) = 0.879)

The obtained results of biological effectiveness represent a good basis for further research into the biological effectiveness of Ni(II) complex towards other plant pathogenic fungi.

Acknowledgements

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P-AgroEnv-07

Valorization of lignocellulosic residues generated in the Valencian Community for environmental applications. The NIRALIG project

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Introduction

The growing trend towards a sustainable and circular economy has promoted the need to look for alternative and environmentally friendly ways to manage waste. Agro-waste produced during harvesting and processing of tiger nut (*Cyperus Esculentus L*), a typical crop in the Valencian Community, is rich in lignocellulosic materials. Lignocellulosic biomass species are basically composed of cellulose, hemicellulose, lignin, extractives and various inorganic materials in a highly complex architecture. The separation of the three basic biopolymers from lignocellulosic biomass is a process of high technological difficulty that is conditioned by many factors, such as the lignin content, the crystallinity of the cellulose, the water content and the available surface area. Due to its high cellulose and lignin content, this waste has great potential to develop smart materials for environmental applications [1]. Specifically, lignin, an aromatic plant polymer, is one of the precursors to the manufacture of intelligent renewable materials, able of responding to different stimuli [2]. The development of new environmentally sustainable extraction processes, such as ultrasound (UAE) and microwave-assisted extraction (MAE), presents great advantages compared to other conventional extraction techniques since they allow more efficient and faster processes, with high potential for their scaling, and showing greater protection of thermolabile constituents, with lower consumption of solvents and energy. All these features are the basic ideas in the NIRALIG project, where residues and by-products obtained from tiger nut will be valorized to obtain new intelligent materials with the capacity to release biofertilizers and/or bioadsorbents of heavy metals in water for agricultural and environmental use.

A new method has been developed to obtain cellulose nanocrystals through microwave-assisted extraction (MAE) based on the processes proposed by Liu *et al* [3]. NaOH and NaClO2/CH3COOH mixture were applied in a FlexiWAVE™ closed vessel microwave unit (Milestone srl, Bergamo, Italy) to remove hemicellulose and lignin. In order to isolate lignin to obtain pure cellulose and lignin fractions, a Box-Behnken design (BBD) was applied with four independent variables (temperature, 80-120 ℃; NaOH concentration, 10-20% (w/v); time extraction, 5-30 min; and solvent volume, 22.5-37.5 mL) at three levels. This design consisted of 29 experiments, including five central points. A comparison with a conventional method of cellulose isolation was also performed. The microfibers obtained after the MAE chemical pretreatment were further hydrolyzed by acid to isolate cellulose nanocrystals (CNC). The final yield of CNC, as well as its crystallinity index obtained by XRD showed better results than those obtained for CNC isolated by the conventional acid treatment. Likewise, the start and maximum degradation temperatures were also obtained by thermogravimetric analysis (TGA); and the analysis of the spectra obtained by Fourier transform infrared spectroscopy (FTIR) and the images obtained by field emission scanning electron microscope (FESEM) also showed the good quality of CNC here obtained. These CNC and the residual lignin fractions will be applied to the development of new intelligent materials with the biofertilizer and/or bioadsorbent of heavy metals performance for agricultural and environmental use

Acknowledgements

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PY-AgroEnv-01

Investigation of deep eutectic solvent-modified oat straw as an efficient adsorbent for Zn(II) ion removal: structural and kinetic study

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Introduction

This study investigated the potential of waste biomass, oat straw (SO), as an adsorbent for Zn(II) removal from aqueous solutions. A selected deep eutectic solvent was used for OS modification (DSO). Structural changes after modification were confirmed by Scanning Electron Microscopy (SEM) analysis. To improve its adsorption properties, the DSO was immobilized into alginate beads, IDSO. The adsorption study was done in batch system. Adsorption capacities of Zn(II) ions removal from aqueous solutions were evaluated for native, modified, and immobilized oat straw. The maximum adsorption capacities for Zn(II) ions were 22.4, 51.4, and 104.78 mg/g for SO, DSO, and IDSO, respectively, indicating a significant improvement of adsorption properties after modification and immobilization of native material. A kinetic study revealed that the adsorption process follows a pseudo-second-order model, suggesting that chemisorption is the rate-limiting step during Zn(II) ion adsorption on to investigated materials. The SEM analysis provided visual evidence of the structural changes induced by DES treatment, correlating with the observed increase in adsorption capacity. These findings underscore the effectiveness of DES-modified biomass in metal ion removal, offering promising insights for sustainable water purification strategies.

Acknowledgements

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PY-AgroEnv-02

Comprehensive studies on cadmium removal in the phosphate fertilizer industry through the adsorption process

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Introduction

Cadmium (Cd) is a toxic heavy metal that poses significant environmental and health risks, particularly in the phosphate fertilizer industry as it can accumulate in soil and crops [1]. This study aimed to investigate a comprehensive method for cadmium removal through adsorption, highlighting the efficacy of commercial resins used to treat industrial wet phosphoric acid (WPA). The research focused on the adsorption mechanism, the influence of operating parameters, and the physiochemical characteristics of the adsorbents in the WPA purification process.

A series of experiments were conducted to evaluate the adsorption capacity of Lewatit K1131 S and Lewatit K1461 cation exchange resins (Lanxess) on Cd(II) ions in crude WPA for phosphate fertilizer production. The batch adsorption studies were designed to determine optimal conditions such as resin dosage, temperature, WPA concentration, initial cadmium concentration, and interaction time to maximize Cd(II) ions removal efficiency. Results indicate that WPA concentration significantly influences adsorption, with higher efficiency observed for lower WPA molarity facilitating surface interaction mechanisms.

Experimental data fitted to pseudo-first-order (PFO) and pseudo-second-order (PSO) kinetic models signifies chemisorption between selected cation exchangers and Cd(II) ions [2]. In turn, Weber-Morris intraparticle diffusion (IPD), and Boyd models indicate that the adsorption process of Cd(II) ions from WPA represents a complex mechanism that includes both intraparticle and boundary layer diffusions [3-4].

Isotherm models, including Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich were employed to analyze the equilibrium data demonstrated that the adsorption of Cd(II) ions onto the selected resins is predominantly monolayer. Under the optimal conditions, the maximum adsorption capacities were found to be 109.17 mg/g, and 172.83 mg/g for Lewatit K1131 S and Lewatit K1461, respectively. The activation energies derived from the Dubinin-Radushkevich isotherm model indicate that the physical adsorption plays a dominant role in the adsorption process of Cd(II) ions on Lewatit K1131 S while in the case of Lewatit K1461 ion exchange occurs [5].

Additionally, the study explores the regeneration capacity of cation exchangers during the desorption process proving their sustainability over five sorption/desorption cycles. Characterization of the adsorbents using techniques such as SEM-EDX, XPS, and FTIR-ATR revealed that surface properties play a crucial role in cadmium uptake, while TG-DTG analysis confirmed the high thermal stability of tested resins.

The findings suggest that the implementation of efficient adsorption methods could significantly reduce cadmium contamination in the phosphate fertilizer industry, contributing to environmental protection and food safety. This research underscores the importance of developing practical and effective strategies for heavy metal remediation in industrial processes, thus promoting more sustainable agricultural practices.

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P-ClimChange-01

Facile hydrothermal synthesis of g-C_3N_4/Cu_3TeO_6 heterostructure with H_2 production photocatalytic properties

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Introduction

In the last years the scientific community has focused on the design and synthesis of novel materials for their application in energy and environmental-related applications [1]. After the pioneering work about water photolysis on TiO_2 electrodes discovered by Fujishima and Honda in 1972, photocatalysis technology has received tremendous attention due to its promising application in H_2 generation [2]. However, the scientific community agrees that it is necessary to develop photocatalysts with adequate redox potential to boost their catalytic activity [3]. Currently, one family of inorganic materials that is drawing the attention of scientists is that of metal tellurates (M_3TeO_6). One metal tellurate that has been studied in several environmental and energy applications due to its interesting electrical, thermal and magnetic properties is Cu_3TeO_6 since this semiconductor can absorb light in the visible range (Eg= 2.6 eV) and presents photocatalytic activity in H_2 production [4]. However, pure photocatalysts exhibit low photoactivity in several applications such as water splitting due to the rapid recombination of photo-induced e^--h^+ pairs and low surface area. In this sense, heterostructure engineering in photocatalysts is a feasible and effective alternative for the spatial separation of e^--h^+ pairs [1-3].

In this work, for first time we developed heterostructures of metal tellurates based on Cu_3TeO_6 with a strong interaction with a well-studied g-C_3N_4 semiconductor to mitigate the drawbacks of this inorganic material. The results obtained by XRD, FITR and SEM showed that the synthesis was successfully developed and that the Cu_3TeO_6 was synthesised on the g-C_3N_4 surface, see Figure 1a. The photoluminescence results showed that the heterostructure presents lower e^--h^+ recombination with respect to the pristine materials, indicating the potential of this heterostructure in photocatalysis. The obtained heterostructure (g-C_3N_4/Cu_3TeO_6) showed photocatalytic activity in H_2 production under UV light (Figure 1b) and a suitable redox potential obtained by UPS and UV-Vis analyses to be a proof of concept for using this novel material in H_2 production applications.

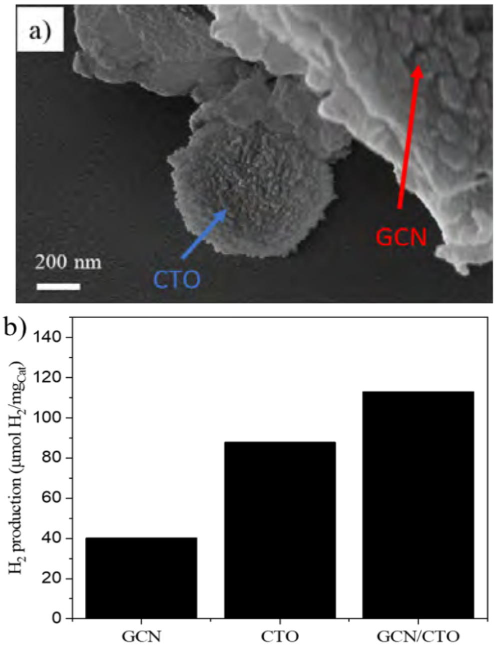

Figure 1: (a) SEM image of the prepared heterostructure samples and (b) H_2 production of the prepared samples.

Acknowledgements

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PY-ClimChange-01

Effects of nitrated monoaromatic hydrocarbons from biomass burning aerosols on chemical composition of the marine microalgae *Dunaliella tertiolecta*

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Introduction

Atmospheric deposition brings organic aerosols, including various organic pollutants, into seawater. An important component of water-soluble aerosols from biomass burning (BB) are nitrated monoaromatic hydrocarbons (NMAHs) [1], which have been shown to have toxic effects on aquatic organisms [2]. Microalgae, the base of the aquatic food web, appear to be very sensitive to the pollution, and the question is how microalgae population will respond to atmospheric originated pollution in their early stages of development.

To investigate the effects of BB aerosols and their NMAHs content on the biochemical composition of the marine microalgae *Dunaliella tertiolecta*, we performed an exposure experiment in a laboratory incubation chamber at controlled nutrient concentrations (f/2 medium), temperature (18°C) and light (4500 lx). The microalgae were exposed to i) the aqueous extract of the particulate matter (PM_{10}) fraction of the simulated BB aerosols (sBB_{H2O}), ii) model NMAHs concentration of 4 µg/L, which corresponded to the amount of NMAHs in sBB_{H2O}, iii) 4 mg/L NMAHs, being 1000 times higher concentration than in sBB_{H2O}. Each incubation and the control were carried out in triplicate. To investigate the very early changes in the particulate organic matter of the microalgae induced by exposure to sBB and NMAHs, sample aliquots were taken several times during the exponential phase of cell growth to analyze abundance, particulate organic carbon, cellular lipids, proteins, carbohydrates and chlorophyll *a* (Chl *a*).

Our results showed a significant decrease in cell growth in all treated samples compared to the control, with the highest growth inhibition (26%) occurring in the culture exposed to 4 mg/L NMAHs. In the same exposure case, analysis of biologically important molecules showed a statistically significant increase in protein/cell on the fourth and seventh day of the exposure. In addition, a significant increase in the cellular concentration of Chl *a* was observed in the samples exposed to 4 mg/L NMAHs compared to the control.

These results suggest that a very high intake of NMAHs, such as mg/L amounts, could be harmful to *Dunaliella tertiolecta* population by affecting their growth and chemical composition. This finding is important since future climate scenarios consider the increased number and intensity of BB events such as forest fires and thus a potential increase of NMAHs in the air and their deposition to the hydrosphere, which could eventually have an impact on primary production in seas.

Acknowledgements

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PY-ClimChange-02

From classroom to consciousness: a hands-on approach to waste management for young students

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Introduction

The curricula for the first cycle of primary schooling in both developed and developing countries worldwide include educational content focusing on the environment, sustainability, and resources [1-3]. Therefore, this paper is aimed to propose an interactive playful exercise (IPE) designed for scholars aged 7 to 12. The IPE is structured around interactive learning methodologies and guided by teacher facilitation, with the goal of familiarizing scholars with topics related to waste generation and its management [4,5].

The task of the teacher is to make a selection of food products (FP), including fresh, canned, and dried fruits, fruit yogurt, candies, and bottled water, packaged in materials such as paper/cardboard, plastic, metal, and glass. Essential tools/items for executing this activity include a digital balance with around 2 kg capacity, cardboard plates and plastic cups for each scholar, and five labeled plastic bags for waste disposal (categorized as Paper/Cardboard, Plastic, Metal, Glass, all referred as Packaging Waste, and Organic Waste). Before consuming the FP (by free choice), scholars are instructed to weigh and record the masses of each FP (including packaging) and the labeled plastic bags, followed by handwashing. After a 15-20-minute period of informal interaction, scholars, guided by the teacher, sort the waste into labeled bags. Before sorting, each scholar individually measures the mass of the waste generated from the FP they consumed. Also, it is necessary for scholars to measure the total mass of each waste category that was created from the consumed FP and record these values in a tabular format. They then calculate the total mass of waste generated relative to the initial mass of consumed FP, exact and average mass of waste produced per person and maximum and minimum mass of waste produced per person. Any unconsumed FP distributed among scholars upon completion of the IPE are factored into the waste calculation.

This activity effectively demonstrates to young scholars the importance of fostering civic consciousness regarding household waste generation, waste types, and primary waste sorting, with appropriate reference to legal regulations [6,7]. The measurements incorporated into the IPE provide a precise depiction of daily waste volumes, reinforcing fundamental mathematical concepts and promoting an appreciation for measurement in real-life situations among scholars. The collaborative problem-solving aspect of the activity emphasizes solidarity, a core principle of civic education. Teachers are encouraged to integrate relevant instruction throughout all stages of the activity.This activity demonstrates the effectiveness of hands-on learning for promoting environmental responsibility among young pupils. Therefore, it is of particular importance to integrate such initiatives into the primary school curricula (ages 7-12), which empowers future generations to become responsible waste managers, at least within their households.

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PY-ClimChange-03

High activity Pd/carbon catalysts prepared from biomass residues for hydrogen production and storage

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Introduction

Hydrogen is an energy vector that is emerging as an alternative to fossil fuels because of their limitations in availability and environmental problems. However, the difficulty with hydrogen remains in its storage by conventional methods [1]. That is the reason why carrier molecules, such as LOHCs (Liquid Organic Hydrogen Carriers) are a very interesting alternative. In this research, we use formic acid (HCOOH) as LOHCs because it presents some suitable characteristics: liquid state at room temperature, low toxicity, easy to store and 4.4 wt % of hydrogen [2]. In addition, it can be directly used for fuel cells, and it is involved in a carbon-neutral cycle with CO_2, where formic acid dehydrogenation and CO_2 hydrogenation take place [3]. Pd supported on carbon materials are the most widely used catalysts for those reactions and interesting results have been achieved with N-doped carbon supports prepared from biomass residues. These materials are frequently synthesized in multiple steps, so that developing simple and environmentally friendly procedures is highly desirable.

In this study, we have synthesized catalysts supported on activated carbon, which is prepared from biomass residues, specifically almond shells. The carbon support was prepared by hydrothermal carbonization (HTC) followed by a thermal treatment at 900 ºC. The effect of the HTC conditions was studied to obtain a highly porous material after the heat treatment. The N-doped counterpart carbon support was synthesised by adding dicyandiamide to the solution used in the HTC, avoiding further steps in the synthetic protocol. Afterwards, Pd-based catalysts (with a nominal metal content of Pd 1 wt %) were prepared by wet impregnation and using $Pd(OAc)_2$ as the metal precursor. Carbon supports were characterized by adsorption isotherms of N_2 at 77K and elemental analysis, indicating that they have an apparent surface area of 1600 m^2/g and that nitrogen was successfully incorporated. Catalysts were characterized by X-Ray Photoelectron Spectroscopy (XPS) and Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-OES). The catalytic activity of these materials was tested in the formic acid dehydrogenation reaction. The results show the positive effect of incorporating nitrogen functional groups into the support, which was confirmed by the better activity and stability of Pd/N-doped carbon compared to the N-free counterpart. This study confirms the suitability of the procedure used for the preparation of the catalysts, which involves less steps than those used in the conventional preparation of these materials, being closer to a green technology.

Acknowledgements

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P-EnvModel-01

Morphological analysis of microplastics revisited – application of pattern recognition and computer vision tools

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Introduction

Since in many routine analytical laboratories a stereomicroscope coupled with a digital camera is not equipped with advanced software enabling automatic detection of features of observed objects, in the current research a procedure of feature detection using an open source software was proposed and validated. Within the framework of the application of microscopic expertise coupled with image analysis, a set of digital images of microplastic (MP) items identified in organs of fish, was used to determine shape descriptors (such as length, width, item area, etc.). Edge points required to compute shape characteristics were set manually in digital images acquired by the camera coupled with binocular, and respective values were computed by the use of built-in MotiConnect software. As an alternative, a new approach was proposed consisting of digital image thresholding, binarization, the use of connected-component labeling, and computation of shape descriptors on pixel level by the use of functions available in an OpenCV library or self-written in C++. 74.4% of images were suitable for thresholding without any additional pretreatment. A significant correlation was obtained between shape descriptors computed by the software and computed using the proposed approach. The range of correlation coefficients at a very high level of significance, according to the pair of correlated measures, was higher than 0.69. The length of fibers can be satisfactorily approximated using a value of half the length of the outer perimeter (r higher than 0.75). Compactness and circularity significantly differ for particles and fibers.

Results obtained confirm that images of MPs acquired by any digital camera connected with binocular can be successfully used to quantify shape descriptors of plastic items by the procedure consisting of digital image thresholding, binarization, determination of connected-component, and computation of shape descriptors on pixel level. Although none of the new image-processing techniques have been proposed, a novelty of the study concerns the use of an open computer vision library or self-written C++ code in unifying the determination of morphological features of MPs detecting in various environmental or biological matrices, which nowadays is of high public interest. As a result, studies on MPs can be worldwide initiated in less equipped facilities.

The proposed approach can be used without any initial preparation of images for those, that present items darker or lighter than the background, however, some additional steps such as dilution, erosion, or application of some histogram-derived thresholding methods could further improve it. The best approximation of the length of the particle can be simply achieved by the computation of the maximal ferret (r = 0.8785), or the longest ellipse axis (r = 0.8443), while the shortest ellipse axis quite well correlates with the width of the MP items (r= 0.8311). An area of items computed by the use of pixel's counting method significantly ($p<0.001$) correlates with the area computed by multiplication of approx-imated length and width of items, however, an approach using the thresholded image analysis enables one to compute precisely also the area of fibers, or shapes possessing slotted holes. Problematic computation of the fibers' length can be overcome by its estimation using the item's outer perimeter length. Circularity and compactness are inversely correlated shape descriptors and diversify particles and fibers. According to our best knowledge, the proposed methodology has not been used in the determination of MPs morphological features as an alternative to more or less user-friendly commercial software. Moreover, a wider range of useful shape characteristics such as outer perimeter length, ferret diameters, or ellipse axes, can be used to qualify MPs of various shapes.

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P-EnvModel-02

Investigation of the effect of sulfates in Fenton reactions in aerosol conditions

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Introduction

Reactions between Fe(II) and H_2O_2, known as Fenton reactions, take place in deliquescent aerosols particles and are regarded as major sources of hydroxyl radicals ($^\bullet OH$) [1]. Atmospheric chemistry models have demonstrated that the high concentration of salts and dissolved organic compounds present in this environment affect the rate constants and oxidant yields coming from these reactions [2]. Because sulfate is a major aerosol component, this work aims to experimentally describe how the Fenton chemistry is affected by the presence of sulfate in aerosol conditions. Hence, the Fe(II) conversion was monitored using the ortho-phenanthroline method, and the radical formation was quantified using Electron Paramagnetic Resonance spectroscopy (EPR) with 5,5-dimethyl-1- pyrroline-N-oxide (DMPO) as spin-trapping agent. Reactions were conducted at pH 3, in 50 mL reaction flasks under a constant stream of nitrogen to prevent parallel reactions between Fe(II) and dissolved oxygen, which are known to occur with faster rates in the presence of high ionic strength (I) [3]. Initially, the isolated effect of ionic strength was investigated in the presence of an inert salt that does not form complexes with Fe^{2+} and does not react with $^\bullet OH$, ClO_4^-. At $I = 4$M, the rate constant of the Fenton reaction showed a decrease if compared to the rate measured in diluted solutions (44.2 ± 1.9 M^{-1} s^{-1}), reaching 24.2 ± 0.4 M^{-1} s^{-1} at pH 3 and 293 K. In the presence of sulfate (SO_4^{2-}, $I = 2.7$ M), the Fe(II) speciation was shifted to $FeSO_4$, and the rate constants significantly increased, reaching 254 ± 10 M^{-1} s^{-1} at pH 3 and 298 K. Spin-trapping analysis revealed that the production of $^\bullet OH$ remained unchanged in the presence of $FeSO_4$ but was notably reduced in the presence of ClO_4^-. This study investigated the Fenton chemistry under conditions typical of aerosol particles, revealing that the reaction rate constant decreases at high ionic strengths, but interactions between iron and sulfate counterbalance this effect and enhances the kinetics of Fenton reactions in aerosols. These findings provide valuable insights which can improve atmospheric chemistry models, such as the Chemical Aqueous Phase Radical Mechanism (CAPRAM) [4].

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P-EnvModel-03

Seasonal PM$_{2.5}$ land use regression models for Novi Sad, Serbia

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Introduction

The urban environment is a key focus for air quality investigations, utilizing various pollution modeling techniques to address significant variability in pollution levels. These models help in assessing the ambient pollutant concentrations and understand their spatial and temporal variability. Particle pollution by PM$_{2.5}$ in Novi Sad, Serbia, is a result of factors like different heating methods (wood, coal, pellet) and traffic, and has been monitored at a few stations at the local and national levels. Within this study, for the first time in Serbia, two PM$_{2.5}$ prediction seasonal (winter and summer) Land Use Regression (LUR) models were developed for Novi Sad.

PM$_{2.5}$ data were sampled on 21 sites in Novi Sad and Petrovaradin municipality during winter and summer by referent gravimetric pumps and microfiber filter replacements were on every 48h. Particle data were used as dependent variables, while data such as land use and land cover, road length, and traffic intensity were used as independent predictive variables needed for the development of seasonal models. Developed models passed evaluation and validation tests and resulted in the creation of PM$_{2.5}$ prediction surfaces for both seasons.

Assessed seasonal winter and summer PM$_{2.5}$ concentrations were in ranges from 25,25-50,21 µg/m^3 and from 10,49-22,31 µg/m^3, respectively. The developed winter LUR model explained 55% of PM$_{2.5}$ variability during the heating season by two predictors, *suburb area* in a buffer of 3.000 m and *total road length* in a buffer of 50 m. *Suburb* was used as a proxy for domestic heating, and *road length* for traffic intensity. Evaluation tests consisted of the determination of Cook's distance, heteroscedasticity, and normality of residuals. Values of Cook's distance were lower than 1 and by White test, it was confirmed that residual variance is equally distributed through measured datasets. Residual distribution for the winter model was treated as approximately normal. Validation was conducted by the Leave-One-Out Cross Validation (LOOCV) method, following adjusted R^2 and RMSE values, which were in the ranges of 34,4-61,3% and from 3,79-4,11 µg/m^3, respectively. Mean absolute error values were from 3,06-3,53 µg/m^3 and values of VIF were between 1,000-1,072. Summer PM$_{2.5}$ LUR model explained 40,3% of PM$_{2.5}$ variability during the non-heating season by one predictive variable, *total road length* in a buffer of 50 m, used as a proxy indicator for traffic intensity as well. Evaluation tests showed the same results as in the case of the winter model with similar ranges. Application of LOOCV method showed adjusted R^2 and RMSE values from 31,2-45,3% and 2,74-3,01 µg/m^3, respectively. Mean absolute errors were from 2,36-2,68 µg/m^3.

The evaluation tests for both seasonal models confirmed that the data structure was suitable for regression analysis, validating the results of both models. The validation results demonstrated the reliability of the PM$_{2.5}$ models for both, winter and summer. The winter model exhibited no multicollinearity, while the summer model had no conditions indicating multicollinearity due to one predictor in the final model. These seasonal models are effective for predicting PM$_{2.5}$ concentrations at unmonitored sites, providing a clear understanding of PM$_{2.5}$ levels within the context of the achieved explanatory percentage of each model. Developed prediction surfaces are a useful tool for future applications of this type of methodology in the sphere of air pollution.

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P-EnvModel-04

Occurrence, dissipation kinetics and environmental risk assessment of antibiotics and their metabolites in agricultural soils

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Introduction

Antibiotics is a group of emerging contaminants of greatest environmental concern due to their capacity to promote the development of antibiotic resistance genes [1]. Their presence in the environment in well-known mainly in aqueous samples, sludges and biota and studies are commonly focused on parent compounds. Nevertheless, to the date there is scarce information about their occurrence and behaviour in soils [2]. This fact is of special concern as antibiotics can end up in agricultural soils irrigated with reclaimed wastewater or fertilizer with treated sludges from wastewater treatment plants. This study investigates the occurrence, sorption, dissipation kinetics, and environmental risk of highly important antibiotics according to World Health Organization (sulfamethazine, sulfadiazine, sulfamethoxazole and trimethoprim) and their main metabolites in Mediterranean agricultural soils [3]. Batch experiments were carried out in a climatic chamber simulating real environmental conditions for 120 days. Five different dissipation models were applied to elucidate antibiotics degradation kinetics: a single first-order kinetic model, a bi-exponential model, a first-order double-exponential decay model, a first-order two-compartment model and a logistic model. The sorption isotherms were evaluated by three different models: Langmuir, Freundlich and linear. Most of the analysed antibiotics and metabolites showed a good fit with the linear isotherm model ($R^2 > 0.96$) and biphasic dissipation kinetic models ($R^2 > 0.90$). The dissipation and the endpoints values (DT_{50} and DT_{90}) depended on the soil type properties. A lixisol type soil demonstrated reduced degradation of the investigated compounds among different studied soils. Trimethoprim showed the highest persistence, followed by sulfamethazine, sulfamethoxazole, and sulfadiazine. Parent compounds exhibited lower degradation rates than their metabolites. The concentrations of the other antibiotics were below their predicted no-effect concentration in soil.

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P-EnvModel-05

Dissipation of endocrine disrupting chemicals in soil: impact of microplastic contamination

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Introduction

Microplastic (MP) pollution has garnered significant attention, yet the interactions between MPs and other organic contaminants in the soil environment remain insufficiently understood. Of particular concern are endocrine-disrupting chemicals (EDCs), which are known for their ability to disrupt hormonal systems in organisms, their persistence, and their widespread presence in various ecosystems. In this study, the dissipation of the most prevalent EDCs was examined in alluvial soil and in soil contaminated with the most found MPs in this environment, namely polyethylene, polyamide, and polystyrene [1]. Batch experiments were conducted under natural conditions in a climatic chamber simulating real environmental conditions for 120 days [2]. The analyses were performed by liquid-chromatography tandem mass spectrometry. Five different dissipation kinetics models were applied to study EDC degradation: single first-order kinetic model, bi-exponential model, first-order double-exponential decay model, first-order two-compartment model and logistic model [3]. Among the EDCs studied, bisphenol A and parabens were the fastest to dissipate, followed by the antimicrobial agents triclosan and triclocarban, with the latter exhibiting limited degradation. Per- and polyfluoroalkyl substances demonstrated high persistence, as concentrations remained nearly constant throughout the experiment. Most compounds followed first-order dissipation kinetics but demonstrated biphasic behaviour. The co-occurrence of MPs in the soil influenced the kinetic behaviour in most cases although the differences were not very marked. MPs may influence sorption and desorption processes, thereby altering the mobility and bioavailability of contaminants to organisms in soil. These findings provide further evidence that MPs can affect the behaviour of soil contaminants like EDCs, not only serving as carriers or sources of pollutants but also influencing their dissipation dynamics.

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P-EnvModel-06

Microalgae meeting with therapeutic muds: the change in organic matter contents and *n*-alkane distributions as a fingerprint for peloid's microalgal enrichment

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Introduction

Peloids (therapeutic muds) represent therapeutic agents formed either *in situ* through contact between the mineral water and the solid phase of geological and/or biological origin (e.g., fine-grained sediments) or are prepared artificially by mixing these components [1,2]. Peloid features depend on the physicochemical characteristics of a solid phase and mineral water, and the duration of mixing between solid and liquid phases, which is known as the maturation ("aging") process [1,2]. Former studies have reported that microalgae may enhance peloid's dermo-cosmetic properties by promoting soothing, regenerating, antioxidant, anti-inflammatory, and antimicrobial effects, improving the skin's performance and benefits [3].

Hence, this study outlines a method for combining a peloid sample with microalgae and mineral water to assess the peloid's enrichment level with microalgal compounds. The enrichment level will be evaluated by comparing the differences in soluble organic matter (SOM) contents and *n*-alkane distributions between the initial peloid and the one mixed with microalgae.

The microalgal biomass used for this experiment consists of several types of microalgae, among which *Scenedesmus* sp. predominates, cultivated in pools for microalgal growth stimulation. Later on, 25 g of the dry peloid from the Bujanovac Spa (BU peloid) was mixed with 2 g of microalgae and ~150 ml of spa mineral water. The mixture was left to sit for six days under ambient temperature and pressure conditions. The SOM extraction from BU peloid (~20 g), microalgae (~7 g), and peloid-microalgae mixture was performed via the Soxhlet extraction method using an azeotropic mixture of dichloromethane and methanol for about 36 h. Next, the saturated hydrocarbon fraction was isolated from the OM via column chromatography and analyzed via gas chromatography-mass spectrometry. For quantitative *n*-alkane analysis, the internal standard (Tetracosane-d50 98 atom % D, Sigma Aldrich) was used. The analysis of *n*-alkanes was conducted utilizing the *m/z* 71 ion chromatogram.

The organic matter (OM) in the initial peloid had a high concentration of long-chain alkanes (n-C_{27}, n-C_{29}, and n-C_{31}) exceeding 500 ppm and a relatively low content of the SOM (485 ppm). In contrast, the microalgal OM indicated a predominance of the short-chain n-C_{17} alkane (over 1400 ppm) and a higher level of SOM (65093 ppm). The n-C_{17} dominated the n-C_{27}, n-C_{29}, and n-C_{31} alkanes in the OM of the 6 days peloid-microalgae mixture (n-$\mathrm{C}_{17} > 1300$ ppm), followed by a significant increase in the SOM compared to the initial peloid (3492 ppm). Even though the added biomass for the experiment was 12.5 times lower than the mass of the peloid, the SOM of the mixture was enriched with microalgal organic matter and n-C_{17} alkane, as the microalgal biomass yielded a concentration of SOM almost 135 times greater than that of the initial peloid.

This preliminary study potentially suggests a systematic enhancement of dermo-cosmetic peloid properties through peloid enrichment with microalgal compounds in a short time frame. However, further experiments are needed to fully characterize microalgal peloids.

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P-EnvMonit-01

Analysis of the total mercury content in soil samples from the city of Lodz in central Poland

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Introduction

Mercury is one of the most toxic naturally occurring elements. It has been widely used in industry, and its diversity and volatility have contributed to its distribution in the natural environment. This poses a threat to ecosystem homeostasis and human health. Both natural and anthropogenic activities contribute to the release of mercury into aquatic and terrestrial ecosystems [1]. Mercury does not biodegrade and circulates freely between the main environmental compartments - air, soil and water [2]. Through the biotransformation process, it enters the food chain and poses a threat to living organisms. Phenomena such as temperature~~,~~ precipitation, wind speed, humidity and ocean currents influence the volatility of an element by limiting or stimulating transport and release and ocean currents [3]. Mercury is released into the atmosphere as a result of manufacturing processes and electricity generation, where it binds to water vapour and dust. However, most of the mercury remains in the atmosphere and has the potential to be transported over long distances. Mercury undergoes several transformations after entering a body of water or soil.

Coal combustion processes in the field of energy production and transformation are the largest source of mercury in the environment in Poland. Despite the slow transition away from coal as the main energy source, Poland still obtains over 60% of its energy from the combustion of hard coal and lignite. Mercury released into the environment undergoes many transformations, including: deposition on land, which can lead to mercury contamination of soil. This in turn leads to mercury entering the food chain through the involvement of microorganisms in the soil. These microorganisms convert various forms of mercury into forms that are available to living organisms, including plants [2].

The monitoring of mercury in soil is an important issue due to the toxicity of mercury, which is a real threat to the environment and human health. Regular monitoring of mercury levels in soil makes it possible to assess changes in the concentration of this element in soil. A study carried out in 26 countries of the European Union showed that the average concentration of mercury in surface soil is about 38 µg/kg. About 10% of the area has concentrations higher than 85 µg/kg, and in some places concentrations are higher than 422 µg/kg.

The variation is influenced by natural processes such as vegetation, temperature and pH, as well as historical mining activities and coal-burning sites [4].

The aim of this work is to correlate the results of analyses for the determination of the total mercury content in soil samples with the place of their collection from different locations in the city of Lodz using the technique of Cold Vapour Atomic Absorption Spectroscopy (CVAAS). Soils from different locations in the city of Lodz in central Poland were the subject of this study. In total, 81 soil samples were analysed. The soil samples were dried at room temperature, sieved and crushed. The total mercury content was measured using MA-3000 automatic mercury analyser from Nippon Instruments Corp. The results obtained are used as a basis for determining the possible source of contamination in the area under consideration. The identification of anthropogenic pollution sources affecting the mercury content in soil samples is important from the perspective of spatial planning and environmental protection activities.

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P-EnvMonit-02

Mercury in air and environmental samples near Europe's largest lignite-fired power plant

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Introduction

Mercury and its compounds are currently on the list of the most dangerous substances for living organisms. The properties of mercury make it a ubiquitous element in the natural environment. It exists in many physical forms and chemicals with a wide range of properties. Biochemical and geochemical transformations between these forms cause the distribution of mercury on local and global scales, as well as its bioaccumulation in living organisms [1]. One of the main sources of high mercury emissions to the environment are coal combustion processes in the energy production and transformation sector. Poland remains dependent on coal and has made very little progress in transforming its energy system. Coal is still the dominant energy source, not only in the power sector but also in the economy as a whole, although its share in the energy mix will fall to a record low of 63% in 2023. n 2010, Poland emitted 14.9 tonnes of mercury per year into the air, currently it is just over 8 tonnes per year, but we are still first in Europe [2]. Mercury contamination, initially considered a serious local problem, is now a global issue. Although present in the environment in trace amounts, mercury poses a serious threat to human health and life due to its high toxicity and ability to participate in various natural cycles. In 2009, the Governing Council of the United Nations Environment Programme began intensive work on a document that would comprehensively protect the environment and human health from the effects of mercury in the environment, the so-called Mercury Convention (Minamata Convention on Mercury). The main objectives of the Convention are to reduce the supply of and demand for the use of mercury in products and technological processes, to prohibit or restrict international trade in mercury, to ensure the safe management of mercury-containing wastes, and to reduce emissions of mercury to the atmosphere and releases of mercury to water and the environment [3].

The largest coal-fired power plant in Europe is located in Poland. The Bełchatów power plant provided about 21% of the national electricity production in 2017. In 2019, almost 60 million tonnes of hard coal and 50 million tonnes of lignite will be mined in Poland. A significant part of the total amount of coal, about 38 million tonnes, was mined in the Bełchatów mine. The main forms of mercury in flue gases from coal combustion are: elemental mercury (Hg^0), divalent mercury (Hg^{2+}) and mercury adsorbed on dust particles ($Hg_{(p)}$) [4]. Mercury and its compounds emitted into the atmosphere are harmful to the environment and toxic to living organisms, mainly due to their transformation in the aquatic environment (through the activity of microorganisms) into so-called methylmercury, which is particularly easy for living organisms to accumulate. Mercury is abundant in coal shale, oil shale, alkaline crystalline rocks and clayey soils and peat. It is a contaminant of fossil fuels. The concentration of mercury in Polish coal seams varies. Analyses of samples of both bituminous coal and lignite show average mercury contents of 0.05-0.20 mg/kg and 0.12-0.45 mg/kg, respectively. A higher mercury content is observed in lignite compared to bituminous coal.

The aim of this study was to attempt to determine the effect of the presence of a power plant on the mercury content of environmental components (bioindicators) and the distance from the source of pollutant emissions on the mercury content of the tested samples. The samples tested were: surface soil (to a depth of 10 cm), bioindicators (mosses, lichens and pine needles) and air samples. Samples were collected in the vicinity of the Bełchatów power plant (directions: east, west, south and north) during the heating season. The MA-3000 mercury analyser was used to determine the content of total mercury in solid samples, while the RA-915M mercury analyser was used to determine the content of metallic mercury vapour.

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P-EnvMonit-03

Geochemical dynamics and risk assessment of potentially toxic metals in irrigated agricultural soils of the Mediterranean region

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Introduction

Healthy, productive, and uncontaminated soils are essential for maintaining balanced ecosystems, ensuring safe food production, capturing carbon, regulating and storing water, enhancing the quality of landscapes, and greening urban areas. Soils across Europe are under threat, the European Commission report “Caring for soil is caring for life” reveals that 60-70% of European soils are unhealthy due to current management practices. Human decisions and actions have led to soil acidification, salinization, sodification, eutrophication processes, and the increase of potentially toxic metals (PTM), pesticides, and other pollutants, accelerating soil erosion and degradation. Due to their properties, PTMs persist in the soils, leading to their accumulation over time. This accumulation can disrupt soil function, degrade crop quality, and ultimately pose risks to human health through the food chain. Several studies have shown that inadequate agricultural practices increase PTM concentrations in soils. So, the objectives of this study were: (i) to assess the level of contamination in agricultural soils from the Alentejo region (South of Portugal); and (ii) to determine soil pollution risk using various indices based on chemical and biological interpretations.

The study was conducted in 10 agricultural soils with annual and permanent crops (S1, S2, S3, S4, S5, S6, S7, S8, S9, S10), from the Brinche-Enxoé hydroagricultural sub-system (Alqueva system; Alentejo region). Samples were collected in five campaigns conducted on T1 and T2 in 2018, T3 and T4 in 2019, and T5 in 2020. T1 and T3 occurred in spring (March/April) at the beginning of the irrigation campaign, while T2, T4, and T5 were carried out at the end of the irrigation period (September/October). Soil physicochemical properties, such as electrical conductivity, pH, and soil organic matter content were determined. The PTM content was evaluated by inductively coupled plasma mass spectrometry (ICPMs). The analysis of the degree of soil contamination by PTM was done by determining pollution indexes, such as Enrichment Factor (EF), Potential Ecological Risk Index (PERI), and Geoaccumulation Index (I*geo*). The physicochemical properties showed that most samples presented a slight alkaline pH (7.7-8.6), and a low percentage of organic matter (0.49-2.97%). Regarding the PTM quantification, the values of Cr, As, and Ni have surpassed the Portuguese limits for the good quality of agricultural soil in several campaigns (Cr: 66.86-76.11; As: 11.21-23.34, and Ni: 37.14-60.75 mg/kg). The EF values, used to evaluate if the concentrations of PTM were from anthropogenic origin, were always lower than 1.5, which points out a natural source. These results were confirmed by Igeo results between -9.61 and -0.42. Relatively to the PERI index, which gives us the biological effect of total PTM concentrations, presented values between 0.01-17.85 indicating a low risk for the ecosystem.

These results indicate that although the concentrations of certain PTMs exceed the proposed limits for high-quality agricultural soils, some of these elevated values are naturally occurring due to the soils being part of the geologically rich Ossa-Morena Zone (OMZ). Moreover, the concentrations did not pose a significant risk to the agroecosystem

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P-EnvMonit-04

Understanding the sources of marine litter in remote islands: the Galapagos islands as a case study

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Introduction

Determining the sources of marine litter is necessary to establish adequate strategies that help in the mitigation of plastic pollution. Plastic bottles are useful tracers of marine litter and constitute the main item stranding on remote beaches in the Galapagos Islands. We collected plastic bottles at 60 remote Galapagos Island beaches from 2018 to 2022 and inferred their sources based on their age and country of manufacture. Based on the OSPAR rating system for PET drink bottles, 76% of beaches were qualified as badly polluted, with > 34 bottles·100 m^{-1}. Bottle densities were highly variable among beaches (range 0.4–1,165 100 m^{-1}) being the highest density found in this study the highest ever reported in a remote beach. Ocean currents played an important role in the dispersal of marine litter in the Galapagos Islands, being the beaches exposed to the Humboldt current the most polluted. Most identified bottles came from Peru (71%), followed by China (17%) and Ecuador (9%). Although most locally-sold products are made in Ecuador, they contribute little to beach litter loads. Polyethylene terephthalate bottles with lid, which are necessary for litter dispersal, represented 88% of all bottles, demonstrating that most of the litter reaching the Galapagos comes from distant sources, mainly from the South American coast. However, the manufacture dates indicate that at least 10% of Peruvian, 26% of Ecuadorian, and all Chinese bottles come from illegal dumping from ships. Reducing marine litter reaching the Galapagos Islands requires tackling litter leakage from land-based sources in South America and regulate illegal dumping from ships ensuring compliance with MARPOL Annex V.

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P-EnvMonit-05

Aqueous ozonolysis of the antiviral drug Umifenovir (Arbidol)

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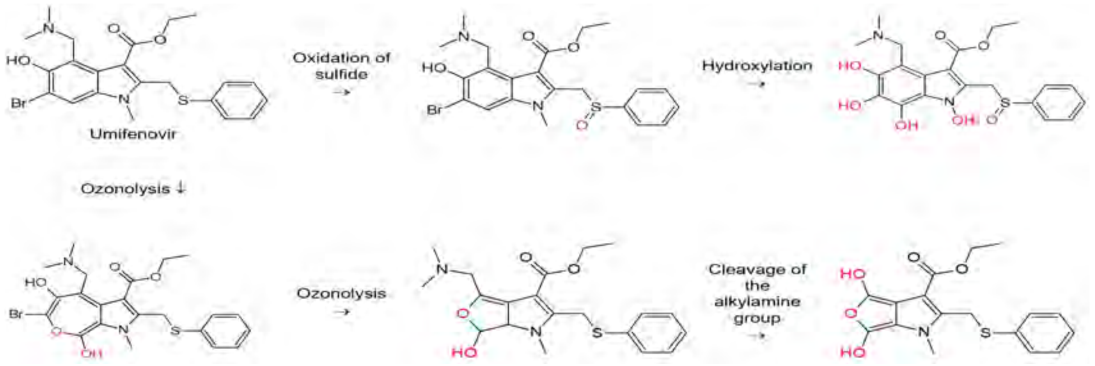
Introduction

Seasonal viral infections and especially epidemics lead to a sharp increase in the consumption of antiviral pharmaceuticals. Among them, umifenovir (Arbidol) deserves special attention due to the large scale of its use in some countries, including Russia and China. It is known that about 40% of the daily dose (up to 800 mg) of umifenovir is excreted from a body unchanged which results in the contamination of municipal wastewaters and natural reservoirs with the potentially hazardous xenobiotic. Currently used technologies of wastewater treatment (disinfection with active chlorine and action of active sludge) do not provide efficient removal of umifenovir and produce unwanted disinfection by-products [1]. A greener alternative to them is the use of advanced oxidation processed and, first of all, ozone treatment (catalytic ozonation). Their development requires deep understanding of mechanisms and pathways of umifenovir transformation under action of ozone.

In this regard, the aim of the present study was to reveal initial interactions of umifenovir with ozone in aqueous media and to identify primary transformation products.

Ozonation of 10 mg/L umifenovir solution was carried out at pH values of 2 and 12 by bubbling ozone at room temperature and continuous stirring. Ozone (10 mg/h) was obtained by passing atmospheric air (200 mL/min) through an ozone generator. The amount of obtained ozone was determined by the iodometric method. The reaction mixture of umifenovir with ozone was sampled at time intervals of 0 (initial sample), 1, 5, 10, 20, 30, 45 and 60 min, a stoichiometric amount of sodium thiosulfate was added to stop the reaction. Sample analysis, search and tentative identification of the transformation products were performed by high-performance liquid chromatography – time-of-flight high-resolution mass spectrometry on a TripleTOF 5600+ Q-TOF mass spectrometer (AB Sciex) combined with Nexera HPLC system (Shimadzu).

The formation of at least 22 main transformation products was established. Their identification was carried out and formation schemes were proposed. While the interaction of umifenovir with active chlorine led mainly to the oxidation of the sulfide group and the elimination of alkylamine moiety, the main directions of transformation during ozonation involve oxidation of the benzene ring (observed at pH 2) and hydroxylation (observed at pH 12). Part of the scheme of Umifenovir transformation during ozonation is given below (Figure).



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P-EnvMonit-06

Environmental Monitoring in the Italian Seas by means of Descriptor 8 of Marine Strategy Framework Directive

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Introduction

ISPRA, on behalf of the Ministry of the Environment, carried out a national environmental monitoring to assess the achievement of GES (*Good Environmental Status*) under Descriptor 8 of the MSFD, ("*The concentrations of contaminants are at levels that do not give rise to polluting effects*") in the three Italian subregions (Mediterranean Sea Region).

In this work the results of the latest six-years (2016-2021), related to chemical contaminants (metals, polycyclic aromatic hydrocarbons, organotin compounds and halogenated organic compounds) in different matrices (water, sediments and biota), are described, using an approach set up on the use of a dimensionless index centred on zero, which allows the evaluation of all regulated contaminants as a whole, for each investigated matrix.

Based on the deviation of the index from zero, chemical quality classes have been established ranging from *GOOD* (deviations absent or within tolerance ranges) to *BAD* (deviation of even a single parameter of at least one order of magnitude compared to the EQS value).

To spatially represent the indexes and class judgment associated, the MRU was divided into GRIDs with different cells dimensions for each matrix.

A judgment on the MRU (*marine reporting unit*) state can be expressed if a spatial coverage equal to at least 50% of the total cells is reached. On the other hand, the GES condition is reached if at least 60% of the surface covered by data is classified as GOOD while the NO-GOOD component (POOR + BAD ratings) does not exceed 25%.

The results showed that Sediments have a high percentage of cells in GOOD state (>60%) even if for the Ionian subregion there was no sufficient coverage to express a judgement. For the Water matrix, although the spatial coverage was poor with data essentially from the coastal area, the situation is encouraging, showing few exceedances related to some parameters such as organotin compounds.

The Biota matrix, instead, presents a NO-GOOD judgement due to the high Hg concentration detected in all areas.

These results are being reported to the European Commission by Italian Ministry of the Environment.

Acknowledgements

Special thanks to all the National Institutions (Environment Regional Agencies and Italian IZS) for their help in environmental sampling, analysis and data sharing.

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P-EnvMonit-07

Biomonitoring phthalic acid esters in marine turtles: sources of contamination and potential implications

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Introduction

Plastic pollution represents a significant planetary threat, with a particularly detrimental impact on marine ecosystems. The pervasiveness of plastics in the marine environment has resulted in ingestion of these materials by a variety of marine organisms. This can occur directly, as observed with sea turtles mistaking plastic bags for jellyfish, or indirectly through the trophic chain. The high prevalence of plastic debris in the gastrointestinal tract of sea turtles has led to the designation of these animals as bioindicators of marine litter [1,2]. One of the most significant adverse effects of plastic ingestion is the potential for chemical contamination of the organism due to the prolonged residence time of the plastic in the gut. This contamination occurs through the uptake of plasticisers, such as phthalic acid esters (PAEs or phthalates) and other toxic compounds accumulated by the plastic and released during digestion. Phthalates have the potential to interfere with the normal processes mediated by hormones, which are essential for growth and development. In addition, the ubiquity of phthalates can be attributed to both anthropogenic contamination and natural origins, as they can be biosynthesised by various organisms, including plants, algae, and bacteria [3].

The objective of this research is to gain a deeper comprehension of the influence of these substances on sea turtles. The concentrations of six phthalates, which were frequently employed as additives, were quantified in diverse tissues and unhatched eggs of sea turtles. The objective was to verify the presence and biodistribution of PAEs in the yolks, albumens, and eggshells, with a view to establishing the origin of contamination.

The HPLC/MS analyses revealed high levels of the most lipophilic phthalates in gonadal and liver samples of *Caretta caretta* and *Dermochelis coriacea* [1]. Furthermore, although to a lesser extent, elevated levels of contamination were also identified in the eggs of *C. caretta* [2].

The statistical analysis confirmed significant differences in the biodistribution of each phthalate and their sum between the eggshell, yolk, and albumen. In light of the potential sources of contamination, a hypothesis is proposed that the phthalates present in eggs originate from the mother, specifically from the release of phthalates during the digestive process. This hypothesis, which is supported by other studies, is further reinforced by preliminary tests carried out on eggshells.

The distribution of different phthalates among tissues allows for the interpretation of the impact that the metabolic pathways of these substances may have on marine organisms.

Acknowledgements

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P-EnvMonit-08

Impact of organic contaminants in soils from Important Bird and Biodiversity Areas

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Introduction

Soil contamination, either from natural or anthropogenic sources, poses a significant threat to biodiversity and ecosystem functioning [1]. In the European Union, the majority of soils are considered unhealthy, with 2.8 million sites identified as contaminated [2]. While research on soil contamination has predominantly focused on urban and agricultural areas, studies in natural environments remain scarce [3]. Filling this gap of knowledge is crucial, as natural areas are key for the conservation of global biodiversity and can play an important role in the retention of contaminants. Furthermore, in the actual context of climate change, the re-emission of persistent compounds from soil is more likely to occur, and in fact, this phenomenon has been already reported in European soils [4]. To assess the health of soils, many countries have implemented long-term surveys focused on metals and organic matter, but lack of harmonized soil monitoring system for organic contaminants, and the real extent of soil contamination, especially for emerging contaminants, is still unknown [5]. In this study, we assessed the contamination status of soils in 140 Important Bird and Biodiversity Areas (IBAs) in Spain. Fifty-two organic contaminants including organochlorine pesticides (OCPs), organophosphorus pesticides (OPPs), polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and plasticizers or plastic related such as phthalates, bisphenol A, nonylphenol, and organophosphate esters (OPEs) were analysed by gas chromatography coupled to tandem mass spectrometry (GC-MS/MS). The mean soil concentration ranged from 1.41 and 917 ng/g and plasticizer and PAHs were detected at the highest concentrations while OCPs were the most frequently detected. Hierarchical Clustering on Principal Components (HCPC) and land use data associated PCBs with artificial land, phthalates with industrial sites and incineration plants and PAHs with burned areas, and in a lesser extent pesticides with agricultural activities. A tier I Environmental Risk Assessment (ERA) was performed to identify the most impacted natural areas and the most concerning compounds. Out of the 140 IBAs, 95 presented at least one compound at high-risk concentrations (RQ>1) for soil organisms. The OPPs chlorpyrifos and malathion, together with the PAH benzo[b]fluoranthene, were detected at high-risk concentrations. Overall, this study highlights the widespread presence of organic contaminants in areas of high natural value and the importance of implementing monitoring studies to identify potential contaminated sites that require conservation and remediation actions for the protection of biodiversity.

Acknowledgements

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P-EnvMonit-09

Assessing Contamination Profiles in Livers from Road-Killed Owls

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Introduction

Biomonitoring programmes that use birds as sentinel species have been proven to be a good approach for the early detection of adverse effects of contaminants in ecosystems and to assess the effectiveness of legislation [1]. Raptors are recognised as valuable sentinel species for monitoring environmental contaminants owing to their foraging behaviour across terrestrial and aquatic food webs and their high trophic position. This study monitored environmental contaminants in livers from road-killed owls to evaluate differences in the exposure patterns due to factors as species, age, and sex of individuals. Carcasses of road-killed individuals of eagle owl (*Bubo bubo*), long-eared owl (*Asio otus*), little owl (*Athene noctua*), tawny owl (*Strix aluco*), and barn owl (*Tyto alba*) were collected in Alentejo (Portugal). Eighty-one organic contaminants were analyzed, including organochlorine pesticides (OCPs), perfluoroalkyl substances (PFAS), polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), pharmaceuticals, in-use pesticides, and organophosphate esters flame retardants (OPEs). Overall, 21 contaminants were detected. ∑OCPs were prevalent in all species at concentrations ranging from 3.24 to 4480 ng/g ww, followed by PFOS, the only PFASs detected (from 2.88 to 848 ng/g ww) and ∑PCBs (1.98 to 2010 ng/g ww). ∑PAHs were ubiquitous but detected at the lowest concentrations (from 7.35 to 123 ng/g ww). Differences among species were observed according to Principal Component Analysis. Eagle owl and long-eared owl presented the highest levels of ∑OCPs, ∑PCBs, and PFOS, consistently with its higher trophic position while ∑PAHs prevailed in tawny owl, barn owl and little owl, related with their frequent use of urban areas for nesting and roadsides for hunting. Additionally, high levels of ∑OCPs, ∑PCBs, and PFOS were observed in woodland species feeding at higher trophic levels, particularly in the eagle owl but also in the long-eared owl. However, these species presented a significantly lower concentration of ∑PAHs than tawny owl, barn owl and little owl. The differences observed can be attributed to more regular foraging in roadsides of the latter species. In general, adults presented significant higher concentrations of ∑OCPs and ∑PCBs than juveniles, while no differences were observed for PFOS and ∑PAHs among ages. Pharmaceuticals, in-use pesticides and OPEs were not detected in any individual. Overall, this study shows specific contamination patterns in 5 species with similar diet but with differences in habitat preferences.

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P-EnvMonit-10

Evaluating an invasive bivalve as a potential environmental proxy for metals in a large South American basin

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Introduction

The shells of mollusks have been widely used as an environmental record because they can incorporate elements from the surrounding environment over time. The aim of this study was to assess the potential use of the *Limnoperna fortunei* shell as a proxy for monitoring the spatial and temporal variability of metals (Ba/Ca, Cu/Ca, Li/Ca, Pb/Ca, Sr/Ca) in fresh and estuarine water. The element/Ca ratios were compared in water samples and bivalve shells proceeding from nine sites of five hydrogeological regions of the La Plata Basin (Argentina and Uruguay), collected in two hydrological periods (winter and summer, 2018) in order to evaluate the chemical composition of the shell as an environmental proxy. Ba/Ca, Cu/Ca, Li/Ca, Pb/Ca, and Sr/Ca were above the detection limit in the shell. Significant positive linear relationships were found between shell edge and water only for Sr/Ca ($R^2 = 0.83\text{-}0.87$, $p < 0.05$) in both summer and winter. No significant relationships were observed for Ba/Ca, Cu/Ca, Li/Ca, and Pb/Ca ($p > 0.05$). These results indicate that the *L. fortunei* shell could be a valuable tool for monitoring spatio-temporal variations in water Sr/Ca shows. However, the shell did not prove to be a good environmental proxy for the rest of the metals analyzed.

P-EnvMonit-11

The Evolving Landscape of PFAS Detection, an Outline of Methods

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Introduction

Perfluoroalkyl substances (PFAS) are a group of man-made chemicals widely used in industrial applications and consumer products. Their widespread usage and resistance to degradation has resulted in PFAS being a ubiquitous environmental contaminant and the potential health effects is of growing concern. While many of the long-chain PFAS have been recognized as harmful, alternative compounds have emerged in their place. Short-chain PFAS compounds are considered to be less bio accumulative and toxic than long-chain PFAS, but their widespread use has resulted in their increased environmental accumulation. In this work, several methods will be outlined to meet the evolving landscape of PFAS analysis. These methods include EPA methods 1633, 533, 8327, and 537.1 as well as a method for the analysis of ultra-short through short-chain (C1-C4) PFAS using a unique hybrid HILIC/ion-exchange stationary phase.

P-EnvMonit-12

A Hybrid Stationary Phase of Ion-Exchange and Hydrophilic Interaction Chromatography for the LC/MS of Polar Compounds

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Introduction

A hybrid ion exchange/HILIC column has been developed for the LC/MS analysis of polar compounds. The phase offers the possibilities of separation of ionic and polar compounds through ion exchange, HILIC or the combinations of both mechanisms, under typical LC/MS mobile phase conditions. Unlike a typical HILIC column, the column reaches equilibrium quickly and reproducibly. The applicability and versatility of the column have been demonstrated by the LC/MS analyses of a wide range of polar analytes. These include the determination of glyphosate and 16 other polar contaminants in food and water matrices, accurate quantification of a large panel of 45 underivatizedamino acids in human plasma, and detection of ultrashort chain and conventional perand polyfluoroalkyl substances (PFAS) in water.

P-EnvMonit-13

Integrated chemical and biological methods for studying the neurotoxic effects of air pollution: application to air samples from Catalonia

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Introduction

Air pollution is one of the greatest environmental risks to health, affecting all people. According to 2019 estimates, air pollution in cities and rural areas around the world causes 4.2 million premature deaths each year, attributed to ischemic heart disease, strokes, chronic obstructive pulmonary disease, acute respiratory infections, and respiratory cancers [1]. However, few studies are exploring the neurotoxic effects of exposure to atmospheric pollutants, despite evidence that fine particles (PM2.5 and PM10) can reach the brain through the bloodstream or olfactory bulb, causing neuronal damage, oxidative stress, and promoting the development of neurodegenerative diseases such as Alzheimer's and Parkinson's.

This study aims to evaluate the neurotoxic effects of atmospheric pollutants in PM10 particles on the SH-SY5Y cell line, a human neuroblastoma model.

A total of 63 samples were gathered over 18 days between January and November 2022 from Air quality samples were collected from four monitoring stations of the Air Quality Monitoring and Prevention Network of the Generalitat de Catalunya, in collaboration with the Public Health Agency of Barcelona. The stations were Bellver de Cerdanya, a rural area in a mountain valley in the Pyrenees; Mollet del Vallès, a suburban area with industrial zones and highways; Manlleu a suburban area with predominant biomass burning pollution and Vic, a suburban area similar to Manlleu, located in the Plana de Vic, prone to thermal inversions that trap pollutants. These samples were analysed using gas chromatography-mass spectrometry (GC-MS) to determine their chemical composition [2]. Biological effects were studied through different assays: cell viability, reactive oxygen species (ROS) production, activation of the xenobiotic response, and acetylcholinesterase activity, a key enzyme in neuronal function.

Thirty organic compounds have been characterized in these samples, including indicators of biomass burning (BB) and incomplete combustion products such as polycyclic aromatic hydrocarbons (PAHs). Winter samples showed distinctive profiles of organic tracers, clearly differentiating them from samples collected at other stations in Catalonia, indicating a higher pollutant load during colder months. Winter extracts from industrial and rural areas such as Bellver, Manlleu, and Mollet del Vallès demonstrated higher toxicity than samples from warmer seasons, reducing cell viability by more than 50%. A significant increase in ROS production and activation of the xenobiotic response were also observed, particularly in winter samples, indicating oxidative stress and activation of detoxifying mechanisms. Additionally, extracts inhibited acetylcholinesterase activity, The most effective samples in inhibiting acetylcholinesterase activity were those from Manlleu and Mollet, with inhibition levels of approximately 35% and 40%, respectively, suggesting a potential neurotoxic risk for population.

These findings underscore the need to develop and implement effective policies to reduce air pollution, especially in areas with high industrial activity or biomass burning. The application of advanced chemical extraction and analysis techniques, coupled with biological studies, is essential for better understanding the risks associated with exposure to these pollutants and their impact on public health.

Acknowledgements

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P-EnvMonit-14

Relationship between total phosphorus, salinity and dissolved oxygen, with *chlorophyll a* in Lagos coastal waters; implication on seasonal eutrophication

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Introduction

Episodic eutrophication evidenced by algal blooms and macrophyte growth, has remained a challenge in Lagos coastal waters, affecting its aquatic health and ability to provide ecosystem services such as transportation, tourism and food for the people [1]. This study aimed to better understand seasonal eutrophication in these waters by investigating the spatial and temporal variations of total phosphorus (TP), salinity, dissolved oxygen (DO) and chlorophyll a (Chl-a), a key indicator of algal biomass [2]. To achieve this, surface water samples were collected for six months during the dry and wet seasons from twenty locations. Total phosphorus and chlorophyll a concentrations were determined by spectrophotometry and multiple linear regression was used to study the relationship of the variables with Chl-a. The observed mean concentration of TP (0.29 ± 0.04 mgL^{-1}) during the dry season was higher than during wet season (0.21 ± 0.04 mgL^{-1}) while the mean Chl-a concentration during the wet season (27.6 ± 5.78 µgL^{-1}) was lower than observed in the dry season (29.9 ± 5.72 µgL^{-1}). The result showed that TP levels have a positive relationship with Chl- a concentration while salinity, on the other hand, showed variable effects, depending on the local water dynamics with higher salinity potentially limiting algal growth in some regions while promoting it in others. Lower dissolved oxygen levels frequently coincided with higher Chl-a concentrations, indicating hypoxic conditions typical of eutrophic waters. These findings further showed that interplay of total phosphorus, salinity, dissolved oxygen and chl-a concentration during the dry season initiated the sporadic harmful algal bloom and growth of macrophytes especially water hyacinth observed during the wet season. This study provides insight into the drivers of seasonal eutrophication in the tropic waters to guide water managers on best management practices for eutrophication mitigation and sustainability of the important waters.

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P-EnvMonit-15

Enantioselective degradation of chiral β-blockers in soil treated with sewage sludge and irrigated with wastewater

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Introduction

The presence of pharmaceuticals as emerging pollutants has been widely reported in the last decades. Pharmaceuticals are mainly released to the aquatic environment through effluent wastewater discharges from wastewater treatment plants, as they are not specifically designed for their removal. Nevertheless, they can also affect agricultural soils irrigated with reclaimed wastewater, which is an increasing practice to overcome the problem of water scarcity [1] or amended with sewage sludge as fertiliser [2]. Many pharmaceuticals are chiral compounds commonly administered in their racemic form, except if one of them is toxic. After administration, their enantiomeric fraction can be altered, not only by enantioselective human metabolism but also by stereoselective biodegradation in specific decomposition processes such as those occurring in wastewater treatment plants [3]. In the last years, there is an increasing concern about the enantiomeric behaviour of chiral drugs in the environment, as they may exhibit different biotransformation, bioaccumulation and ecotoxicity [4]. Nevertheless, to the date there is scarce information about their enantiomeric behaviour as their analytical determination is commonly difficult to overcome in complex environmental samples [5].

This study is focused on the behaviour and dissipation kinetics of the enantiomers of chiral β-blockers, a therapeutic group of concern due to their long-term and extended use to treat several chronic diseases [6], in compost-amended soils, digested sludge-amended soils and in wastewater-irrigated soils. Selected β-blockers were three widely used compounds (atenolol, metoprolol, and propranolol). The few studies that have investigated the degradation kinetics of these β-blockers in soils did not distinguishing the behaviour of each enantiomer. Analytical determination was carried out by a previously reported method [6]. Degradation studies were carried out in quintuplicate for 120 days. Results revealed that atenolol enantiomers exhibit rapid degradation, with complete dissipation within eight days fitting to a first-order degradation kinetic. Metoprolol and propranolol were more persistent and fitted better to biphasic and lag phase kinetic models, respectively. Differences were also found in the degradation kinetics of propranolol enantiomers. The highest degradation was observed in digested-sludge amended soils and the lowest in compost-amended soils.

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P-EnvMonit-16

Matrix solid-phase dispersion for determination of tetracyclines in solid environmental samples

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Introduction

The presence of antibiotics in the environment has been widely reported for many years. Tetracyclines, broad-spectrum antibiotics, are widely used to treat diseases in both humans and animals. They are among the most commonly used antibiotics for treating bacterial infections and as feed additives to promote growth in aquaculture and animal husbandry [1]. Despite the persistent presence and impact of tetracyclines in the environment [2], data on their occurrence in solid environmental matrices remains insufficient, partly due to the lack of reliable analytical methodologies for their determination in such complex matrices.The ability to accurately quantifying these antibiotics in complex matrices is essential for evaluating their environmental fate and potential risks. The analytical methods described for the determination of tetracyclines in environmental solid samples are multiresidue analyses which include a short number of tetracyclines. They are usually based on solid-phase extraction (SPE) [3]. The matrix solid-phase dispersion (MSPD) technique is a promising alternative to SPE due to its efficiency in integrating the extraction and clean-up steps into a single process. It also offers the advantage of miniaturisation, facilitates sample preparation, as it requires smaller sample amounts, and has provided good results when applied to different analytes and matrices [4]. MSPD involves assembling cartridges where the sample mixture, previously dispersed with a dispersant sorbent, is introduced.

The aim of this work is to propose an analytical method for the determination of seven tetracyclines; tetracycline, 4-epitetracycline, oxytetracycline, epioxytetracycline, chlortetracycline, doxycycline and methacycline, in sewage sludge, composted sludge, and soil. The method is based on the extraction of the compounds from the solid matrix by MSPD, followed by determination by liquid chromatography-tandem mass spectrometry (LC-MS/MS). The method was optimised in terms of type and ratio of dispersant, type of elution solvent, number of extraction cycles and sorbent used for extract clean-up. To better evaluate the interactions between the variables, Box-Behnken experimental designs were employed in the optimization process. Recoveries were above 60% for most compounds, with precision, expressed as relative standard deviation, lower than 15%. Detection limits generally below 80 ng g^{-1} dry matter. Matrix-matched calibration curves were used for quantification. The applicability of the method was verified by analyzing sludge, compost, and soil samples.

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P-EnvMonit-17

Employing Cutting-Edge Methodologies for In-Depth Spatiotemporal Analysis of Water Quality Dynamics in Serbian Rivers

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Introduction

The Danube River in Serbia is confronting significant pollution challenges, particularly near major urban and industrial centers such as Belgrade and Novi Sad. Current monitoring systems provide insufficient insight into the temporal and spatial fluctuations in water quality. This study, covering the period from 2011 up to 2022, aims to identify pollution hotspots and elucidate the factors influencing water quality. Data from 12 localities along the Danube and Tisza Rivers were analysed using hierarchical cluster analysis (HCA) to uncover pollution patterns across 19 physical and chemical parameters.

Key findings indicate that Bezdan, Novi Sad, and Bogojevo on the Danube consistently exhibited elevated contamination levels, while Novi Bečej and Titel on the Tisza were also notably affected. An expanded dataset incorporating six additional localities identified Zemun and Novi Sad additionally, as the major pollution hotspots. The analysis revealed untreated municipal and industrial wastewater as primary pollution sources, highlighting the need for targeted remediation efforts.

The study further examined the impacts of seasonal, meteorological, and anthropogenic factors on water quality. Variations in industrial discharges, agricultural runoff, and weather patterns were found to significantly influence fluctuations in water temperature, dissolved oxygen, and nutrient levels. To improve measurement accuracy, a novel mobile sensor system was deployed along the Danube and Sava rivers, capturing over 7,700 real-time data points for key parameters. This system, which included measurements in segments such as Marina Dorćol and Marina Zemun, demonstrated significant oscillations in conductivity, driven by both, natural cycles and pollution sources.

Comparative analysis with stationary SEPA data [1] underscored discrepancies, illustrating the enhanced effectiveness of mobile monitoring in capturing spatial and temporal dynamics of water quality. Specifically, our measurements were compared with data from SEPA's Zemun station, revealing that, while SEPA classified the Danube as Class I water, our data suggested Class I based on conductivity, but Class V based on pH and oxygen levels. This classification indicates a poor ecological status, implying that the surface water is unsuitable for any use.

The observed variations may stem from several factors, including the upstream location of SEPA's Zemun station relative to our monitoring sites and the stationary nature of SEPA's measurements compared to our mobile, high-resolution data. This study emphasizes the necessity of implementing continuous, high-resolution monitoring systems to identify and mitigate pollution sources effectively. Such systems will facilitate a more precise understanding of water quality dynamics and support targeted environmental management strategies to safeguard the ecological health of the Danube River.

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P-EnvMonit-18

Implementation plan to monitor microplastics in surface and drinking water according to Directive (EU) 2020/2184: Barcelona case study

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Introduction

The increasing prevalence of microplastics (MPs) in freshwater environments, particularly in rivers and groundwater, has become a major concern in recent times [1]. Although drinking water treatment processes are generally effective at removing microplastics, they can reach drinking water [2], potentially compromising its quality.

In this study, a sampling and analytical design based on pyrolysis-gas chromatography coupled with mass spectrometry (Py-GC-MS) were proposed to determine the six main types of microplastics: polyethylene terephthalate (PET), polyethylene (PE), polyvinyl chloride (PVC), polypropylene (PP), polystyrene (PS), and polycarbonate (PC) in surface water samples collected along the Llobregat river basin, the main source of raw water for drinking water production in Barcelona area. In addition, the drinking water supply network of the metropolitan area of Barcelona was also monitored, including most of the distribution areas of the network.

In the Llobregat river and its tributaries (n=17), ΣMPs increased downstream to 544 µg/L at the inlet of the Sant Joan Despí drinking water treatment plant (DWTP). Most of the MPs were eliminated during the water treatment process and were detected at an average concentration of ΣMPs of 0.49 µg/L in 43% of the drinking water network. PE and PVC were the main polymers detected both in the surface water and in the drinking water supply network, followed by occasional detection of PS and PP. The proposed strategy aligns with Directive (EU) 2020/2184, which lays down the methodology for measuring MPs in water intended for human consumption.

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P-EnvMonit-19

Health Risk Assessment of Rare Earth Elements in Road Dust near Coal-Fired Thermal Power Plants

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Introduction

Road dust is a major source of fine and ultrafine particles from the atmosphere which contains elements that originate from past industrial activities, combined with particles from asphalt, road paint, tires, brakes, and car parts [1, 2]. Rare earth elements (REEs) are among the constituents of road dust that may have negative effects on human health [3].

Samples of road dust were collected from 17 locations (both main and side roads) within a 15 km radius around two coal-fired thermal power plants (TPP Kostolac, Serbia). The concentrations of nine REEs (Sc, La, Ce, Nd, Sm, Eu, Tb, Dy, Yb) were measured in the road dust samples (fraction size $f < 63$ µm, easily resuspended) using Instrumental Neutron Activation Analysis (INAA).

To assess the potential health risks posed to humans by toxic elements, including REEs in road dust treated as soil samples, a health risk assessment (HRA) model was used [4]. The chronic daily intake (CDI) and ingestion rates (adjustable) IR_{adj} are computed for both adults and children exposed to potentially hazardous REE from the dust samples. For overall health risk assessment from REEs in analyzed road dust samples the hazard index (HI) was calculated as the sum of each REE hazard quotient HQ.

Our findings showed that REE concentrations were not influenced by the distance of the sampling site from the Thermal Power Plant. Based on a hazard index below 0.1, the road dust samples in the tested area do not pose any significant risk to human health. Although the overall risk was low, slight variations were observed in the hazard quotients of two REEs (Eu and Dy) when comparing the results from two different sampling campaigns.

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P-EnvMonit-20

Selenium speciation in the aqueous samples of old Salsigne mining area (Aude, France)

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Introduction

Sulfide mining environments often contain elevated concentrations of iron (Fe) and sulfur (S), which can significantly influence the solubility and speciation of selenium (Se). Redox gradient conditions, common in these environments, can favor predominance of mobile and soluble Se(VI) and Se(IV) species Se under oxic conditions, while anoxic conditions promote Se precipitation as metal selenides or elemental Se [1]. However, the mechanisms by which Fe and S interact with Se in mine drainages remain poorly understood [2].

This study investigated Se speciation in the surface waters of the Orbiel watershed, which drains mining wastes in the Salsigne area, France. An adapted HPLC-ICP-MS analytical technique was used to determine Se(IV), Se(VI), and SeCN species at low total Se concentrations [3]. Various preservation approaches were evaluated to assess oxidation risks and ensure accurate Se speciation. Additionally, physico-chemical parameters such as pH, Eh, conductivity, O_2 concentration, geochemical composition, major ions, dissolved organic carbon (DOC), and the speciation of key redox-sensitive elements (Fe^{2+}/Fe^{3+} and S^{2-}) were analysed.

Overall, Se(VI) species were found to dominate in the pool of inorganic Se species (Se_{inorg}) under the oxidizing conditions. However, in majority of samples in which Se speciation analysis was performed, fraction of Se_{inorg}. was substantially lower than the determined Se_{TOT}. This is especially observed in the resurgences to the Orbiel and can reflect unknown mechanism of complexation of Se in the dissolved phase. At the station characterized by reducing conditions and high Fe^{2+} and S^{2-} concentrations, the lowest concentration of total Se was determined, and SeCN species were dominant. Thus, data suggest that high Fe and S concentrations under reducing conditions promote Se removal from the dissolved phase, while organic species seem to be stabilized in the dissolved phase.

This study highlights the significant influence of redox gradient conditions on Se solubility, speciation, and biogeochemical cycling in sulphide mining environments. The precise mechanisms of Se interaction with Fe and S, as well as other complexation processes in these systems, require further investigation, particularly through solid-phase analysis to identify potential Se-bearing precipitates, in order to better understand the processes occurring in these unique natural environments.

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P-EnvMonit-21

Mineral composition of soil as an indicator of the geographical origin of single-varietal wines

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Introduction

Due to the immense worldwide popularity of wine and its presence in the daily diet of many consumers, there is a need for constant control of both the raw materials, the various stages of production and the final product itself. The elemental composition of wine is determined mainly by its geographical origin, which directly correlates with the composition of the soil. It is believed that 86% of the metal content in wines can be explained by the elemental composition of the soil in the vineyard. This concept is often referred to as “terroir,” which encompasses not only the soil, but also the climate, topography and other natural factors that affect the vines and the final taste of the wine. The chemical composition of the soil affects which minerals and elements are absorbed by the plant, which in turn shapes the character of the wine [1,2].

In the present study, the elemental composition of 246 wine samples was characterized in order to find correlations with viticultural area. The concentrations of 27 elements were determined using the ICP-OES technique. In addition, the pH values of each of the tested wines were measured. The analyzed sample set consisted of 159 dry red wines of the Cabernet Sauvignon varietal, 27 semi-dry red wines of the Cabernet Sauvignon varietal and 60 dry red wines of other varietals (Primitivo, Syrah, Merlot, Monastrell). The alcohol samples came from 19 countries (Argentina, Australia, Bulgaria, Chile, China, Spain, France, Germany, Greece, India, Israel, Lebanon, Moldova, Hungary, South Africa, Romania, Uruguay, USA, Italy - 6 continents (Africa, North America, South America, Australia, Asia, Europe). Information about the mineral composition of soils from grape-growing areas (as declared by the producer) was taken from literature data.

Australian wines were characterized by significantly higher contents of elements such as Fe, Sr and Mn. The source of their origin is absorption from the soil and agrochemical treatments applied. Lateritic soils covering most of Australia are a strongly acid reaction in the surface layer, an intense brick-red color and high concentrations of elements such as iron, manganese and strontium [3]. Italian wines were characterized by the highest calcium contents and high pH values. These results correlate with the characteristics of soil in the wine-growing areas. Limestone soils contain a lot of calcium carbonate, which affects the soil pH, making it more alkaline [4]. In contrast, the highest concentrations of sulfur were recorded in wines exported over long distances (e.g. Chile). Sulfur dioxide is commonly used in winemaking as an antioxidant and preservative to prevent oxidation and the growth of microorganisms [5].

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P-EnvMonit-22

Monitoring of trace element levels in soil from areas surrounding highways and expressways in the Lodz region in Poland

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Introduction

Urban soils accumulate pollutants, such as toxic elements, from a variety of anthropogenic sources [1-2]. One of the largest sources of heavy metals, including platinum group metals (PGEs) are vehicle emissions. As heavy metals including platinum group metals are omnipresent, their negative impact on human health is very likely. Due to their long biological half-life and high toxicity, they tend to accumulate in the environment. Platinides can impair important biochemical processes, posing a threat to the health and life of humans, animals and plants. Human activities have contributed to the disruption of the biochemical and geological cycles of heavy metals and PGE. The emission of harmful substances, including toxic elements, has become a worldwide environmental problem in urban areas since the rapid development of industrialisation and urbanisation [2]. In this context, the Lodz region and the city of Lodz, as a post-industrial city with a rich history of dynamic development of the textile industry and increased transport, is a prime example of an area particularly vulnerable to soil pollution. The city's central location in the country plays an important role in interregional and international transport as one of the main transport junctions in Poland (the course of two motorways A1, A2, express road S14 and the western bypass of Lodz - road S8, the presence of a developed railway and an airport) [4]. Undoubtedly, direct characterisation of soils in relation to toxic element pollution can potentially be used as an effective scientific tool for diagnosing sources of pollution [1-3]. Nowadays,the combination of geographic information technology (GIS) with geostatistical techniques and multivariate chemometric analysis is increasingly used in studies on heavy metal pollution of selected regions. As a result of combining several approaches, the results obtained and their appropriate interpretation may have important implications for the development of strategies and policies aimed at preventing widespread heavy metal pollution [3].

In the present study, based on tests performed by the following techniques: ICP-OES (e.g, Cd, Cr, Cu, Ni, Pb, Zn, Fe), AAS (Hg, Pt, Pd, Rh), an attempt was made to determine the variability of toxic element levels as the degree of contamination of the soil samples studied using a systematic sampling strategy and a common methodology. In this study, 65 sampling points from the Łodzkie region near roads with heavy traffic (A1, A2, S18, S14), located in central Poland, were investigated. Soil samples were taken at each point, taking into account the depth of soil layers sampled and the distance of the point from the selected road. Preparation of soil samples prior to quantitative analysis by ICP-OES and AAS techniques included drying of soil materials, sieving and grinding in a porcelain mortar. Weighed samples (approximately 0.3 g) were treated with a mixture of 4.5 ml HNO_3 (Baker) and 1.5 ml HCl (Merck). After decomposition in an UltraWave closed microwave energy system (Milestone), the samples were transferred to 50 ml flasks and centrifuged using an OHAUS centrifuge. In addition, optimisation of the decomposition parameters was carried out using certified reference materials. Different reagent ratios and sample mineralisation conditions were tested. An additional aim of the study was to confirm the usefulness of the applied statistical tests and multivariate analyses (STATISTICA ver. 12.5) and geographical information systems (Esri ArcGIS Pro 3.0.3) in identifying the influence of spatial variability on the elemental composition of the studied samples. The results obtained in the project can be used to assess the degree of contamination of soils with heavy metals, including PGE elements, and provide a basis for further monitoring to assess changes in their levels in the future.

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P-EnvMonit-23

Hydrochemical and Isotopic Characterization of the Waters in the Upper Basins of the Llobregat and Cardener Rivers

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Introduction

Currently, many river basins are experiencing critical water stress, particularly because of global change, as is the case in Catalonia (Spain). The analysis of stable isotopes and hydrochemistry is a valuable tool for understanding the hydrogeological cycle at both regional and local scales, and therefore, the origin of recharge. Identifying hydrogeological functioning is essential for public administration, as it allows for optimal and sustainable short- and long-term management, as well as defining management and consumption strategies in the face of climate change.

The study area corresponds to the upper basins of the Llobregat and Cardener rivers, which feature a complex karst system with faults and thrusts, resulting in the Cadí-Moixeró mountain system. The objective of this study is to characterize the waters (precipitation, springs, groundwater from piezometers, and surface water) of the three aquifer systems present in the study area: the aquifer of conglomerates, marls, and Mesozoic and Paleogene limestones of the Cadí-Llobregat; the aquifer of Devonian limestones of Moixeró; and the aquifer of Mesozoic and Paleogene limestones, conglomerates, and marls of Pedraforca-Llobregat. To achieve this, a series of sampling campaigns were conducted throughout 2024, analyzing stable water isotopes, major and trace elements in the water, establishing the relationship between different water types, and estimating the back trajectories of moisture masses that caused the precipitation collected and analyzed.

In general, almost all the waters analyzed in this study are calcium-carbonated water with low mineralization (below 10 meq/L), with a few exceptions. On the other hand, when comparing the stable isotopes of the samples collected in each campaign, it is observed that the waters collected in the fourth campaign (from May 17 to June 19) are more enriched in heavy isotopes than those from the first campaign (from April 8 to April 12, 2024). When analyzed by water type, the water most enriched in heavy isotopes corresponds to precipitation (average δ18O = -5.77 ± 1.58‰; average δ2H = -33.29 ± 11.61‰), followed by groundwater taken from piezometers (average $\delta^{18}O$ = -8.39 ± 0.62‰; average $\delta^{2}H$ = -53.51 ± 4.81‰), then springs (average $\delta^{18}O$ = -8.62 ± 0.64‰; average $\delta^{2}H$ = -53.76 ± 4.38‰), and the most depleted in heavy isotopes is surface water (average $\delta^{18}O$ = -8.40 ± 1.92‰; average $\delta^{2}H$ = -51.54 ± 11.71‰). This reflects that the recharge area corresponds to higher altitudes than those analyzed in this study, as shown by the isotopic composition of precipitation [1].

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P-EnvMonit-24

Electrochemical Biosensing of Alkaline Phosphatase Inhibitors

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Introduction

Marine pollution is a problem concerning most of the planet's areas today. Substances that generate environmental issues are mainly anthropogenic, such as biocides, heavy metals, organochlorine compounds or polycyclic aromatic hydrocarbons. Furthermore, inorganic fertilizers coming from agricultural discharges, such as phosphates, nitrates, or ammonium, lead to eutrophication phenomena that seriously affect ecosystems. The present study aims to develop an electrochemical indirect monitoring biosensor based on enzymatic inhibition in order to detect pollutants in seawater.

Currently, enzyme-catalyzed processes are increasingly used in areas such as health, environmental protection, pharmaceutical research, and food safety, among others. These processes exhibit high catalytic activity, high substrate specificity, and are active at room temperature, atmospheric pressure, and neutral pH. Therefore, enzymes are a widely used element in the manufacture of biosensors, due to their high specificity and selectivity.

For the development of biosensors, the immobilization of the enzyme is fundamental, since it improves the stability of the enzyme, in addition to the possible reuse of the derivative, the easy handling and control, allowing the diffusion of substrates and inhibitors through them. A good method to encapsulate enzymes is the silica matrix synthesized by the sol-gel method, it is a good method since it can be molded, this makes it a suitable method to modify electrodes, and the chemical reactions occur under mild conditions. To modify the porosity and to improve physical properties such as the accessibility, silica can be modified with organic groups, driving to ORganic MOdified SILica (ORMOSIL).

This work presents a study on the incorporation and characterization of the enzyme Alkaline Phosphatase (ALP) in conventional silica matrices synthesized by the sol-gel method and in ORMOSIL. ALP was immobilized by a two-step sol-gel methodology and the properties of the encapsulated enzyme were compared with those obtained in solution. Conformation and stability were analyzed by monitoring changes in the intrinsic fluorescence of the protein as a function of temperature to understand the unfolding/folding process within the sol-gel, which is closely related to enzyme activity. The results reveal that the immobilized enzyme retains its activity.

Hydroquinone diphosphate (HQDP) was used as substrate, since its enzymatic hydrolysis produces hydroquinone (HQ), an electroactive product whose formation can be easily detected by cyclic voltammetry. In a first step, a kinetic study was used to determine the enzymatic activity towards HQDP hydrolysis. The presence of different organic moieties in the ORMOSIL may affect to the access of the substrate/products within the silica pores and also to the structural state of the encapsulated enzyme. The effect of the organic group on the catalytic activity of the enzyme was explored, in order to obtain fast responses for the future development of a suitable biosensors.

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P-EnvMonit-25

Preconcentration of selected cephalosporins using waste pet-derived UIO-66 as an adsorbent before HPLC-DAD quantification

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Introduction

The widespread use and misuse of cephalosporin antibiotics are leading to their alarming presence in water sources like groundwater, surface water, and soil, posing significant threats to both the environment and public health [1–3].In this work, a method for the extraction, preconcentration and determination of five different cephalosporin antibiotics in various water samples using ultrasound-assisted dispersive solid-phase extraction (UA-DSPE) and high-performance liquid chromatography coupled with diode-array detection (HPLC-DAD) was developed. The waste PET-derived UIO-66 was used, prepared, and characterised using Fourier transform infrared spectroscopy, X-ray diffraction, high-resolution scanning electron microscopy, transmission electron microscopy and energy dispersive X-ray spectroscopy. The large surface area, pore volume, and microporous nature of the material were necessary to ensure there were abundant active sorption sites for the cephalosporin antibiotics (cefoperazone, ceftriaxone, cephalothin, cefaclor and cefoxitin). The factors affecting the UA-DSPE method were optimised using a central composite design. Under optimised conditions, wide linearity ranging from 0.1-700 µg/L with the determination coefficients from greater than 0.99. The limits of detection and quantification were in the range of 0.026-0.096 µg/L and 0.09-0.32 µg/L. The intraday and interday spiked recoveries were 71.4-99.3% and 72.6-99.1%, with the relative standard deviation values less than 6%. The UA-DSPE/HPLC-DAD method was successfully applied to real environmental samples such as wastewater and surface water. The performance of the waste PET-derived UIO-66 material was investigated using a series of adsorption experiments. The adsorption isotherms and kinetics indicated that the pseudo-second-order kinetic model and Langmuir isotherm model explained the adsorption process. The maximum adsorption capacities for the target analytes using waste PET-derived UIO-66 ranged from 68.3-106 mg/g. These results demonstrated that the waste PET-derived UIO-66 material can be used as a sustainable adsorbent for the removal of antibiotics via adsorption processes.

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P-EnvMonit-26

Can SVOC levels in pine needles from different species be comparable?

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Introduction

This work aims to be a starting point to reduce an important gap. That is, to obtain valid relationships between the uptakes of different pine species towards given pollutants while strengthening the knowledge of the levels and cycles of pollution. To achieve these purposes, samples of pine needles from several species were collected in 12 sites from different countries (Portugal, Spain, UK and Romania), where at least two species were planted under a similar environmental exposure (next to each other). A multi-residue analytical protocol previously validated by our group [1] was employed to extract and quantify four classes of semi-volatile organic contaminants (SVOCs) - polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs) and organochlorine pesticides (OCPs) – in order to establish initially the differences between the levels of the target chemicals between them, and then try to produce correlations between pine species for as many compounds as possible. In general, the levels of the target compounds found in the samples reflected the urban pressures, regardless of the species. Some indications point towards a *P. pinaster* > *P. sylvestris* > *P. pinea* > *P. radiata* > *P. halepensis* > *P. strobus* > *P. canariensis* trend of their uptake ability. In the most sampled species, it was possible to establish statistically significant relationships ($p>0.05$) for the sum of concentrations of the different classes of SVOCs and for some of the individual compounds, especially for the most volatile ones and between *P. pinaster* and *P. pinea* and also *P. sylvestris* and *P. pinaster*. These uptake correlations seem to be transversal to the land uses (urban, rural, remote).

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P-EnvMonit-27

Comparing elemental composition of bumblebees to honey bees as biomonitors of metals

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Introduction

Honey bees (*Apis mellifera*) are often used as bioindicators in environmental studies due to their wide distribution and social behavior, which facilitates the collection and analysis of samples. Each forager completes about 15 trips per day. They forage over large areas, usually up to 7 km^2, and sample various environmental compartments, including air (PM), water, soil (through pollen and nectar). Research has shown that honey bees accumulate metals and metalloids, reflecting the level of pollutants in their environment [1].

Bumblebees (*Bombus terrestris*) are native pollinators in Europe that live in colonies with up to 500 individuals. They usually forage from several hundred meters to a few kilometers from the nest. They make more than 10 foraging flights per hour. They can forage at temperatures above 7 °C which makes them active earlier in the year or in colder climates compared to honey bees, who need temperatures above 12 °C. Bumblebees were used as biomonitors of metal pollution in the environment only once until now [2].

The aim of this study is to comprehensively compare the elemental composition of honey bees and bumblebees as biomonitors of metal pollution. Bumblebee hives (each with queen, ~ 50 workers and brood) were placed near existing honey bee hives in an urban region in Aachen, Germany. Individual honey bees and bumblebees were sampled, but into plastic containers and frozen. Samples were kept in at − 26 °C until analysis. From each bumblebee hive four bumblebees were sampled and from each honey bee colony seven honey bees were sampled

Honey bees and bumblebees were dried for 16 h at 105 °C in a drying oven. Afterwards, individual honey bees or bumblebees were digested using an ultraCLAVE IV microwave digestion system with 2 mL conc. HNO3 and 3 mL ultrapure water. The digested solutions were diluted with ultrapure water to contain 10% (*v/v*) nitric acid. All element concentrations were determined using inductively coupled plasma mass spectrometry - ICPMS (Agilent ICPMS 7700x). For thirty-one elements an external calibration curve in four different concentration ranges and with six points each, was made in 10% HNO_3.

Bumblebees are larger in size, and consequently have higher average weight of 137 ± 44 mg, compared to honey bees whose average dry weight was 56 ± 16 mg. Out of all the analyzed elements Li, Ni, Ag, Tl, Pb and U were below the limit of detection (LOD). We observed that there were no statistical differences in element concentration between different hives of honey bees or bumblebees. For half of the elements, we analyzed there were no statistically significant differences between honey bees and bumblebees. These include B, Na, Mg, P, V, Cr, Mn, Fe, Co, Sr, Sb. These include some of the known essential elements for honey bees, such as Na, Mg, P, Fe, Mn, Co and Cr. Considering they are essential it is understandable that both bumbles and honey bees need them in the same amounts. Bumblebees had higher concentration of S, Cu, Zn, As, Se, Mo and Ba compared to honey bees. Higher concentrations in honey bees compared to bumblebees can be observed for Al, K, Ca, Rb, Cd, Sn and Cs. Bumblebees and honey bees visit mostly different spectra of flowers during their foraging activities. This can explain the differences in element concentrations between these two species.

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P-EnvMonit-28

INCOME – Inputs for a more sustainable region: Tools for managing metal-contaminated areas

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Introduction

In the newly introduced European Union (EU) Soil Strategy for 2030, medium- and long-term objectives are outlined, to achieve good soil health. The EU Soil Strategy for 2030 will undoubtedly mandate that all Member States independently develop methodologies for assessing the risks of soil contamination, identify contaminated sites, and establish conditions for the remediation of sites that pose a risk to human health or the environment.

Mining areas are examples of historic contaminated sites where polluters can no longer be held responsible for remediation costs. In Portugal there are around 199 abandoned mines, identified by EDM (Empresa de Desenvolvimento Mineiro, S.A.) since 2001. São Domingos is perhaps, the most representative area in Portuguese territory of IPB (Iberian Pyrite Belt) sector, with a large pit (122 m deep), left open after the extraction works (1857-1966), which now it is filled with acid drainage waters (ADW). This contamination is a latent environmental problem, since the mine area is located along a water line connected with Chança River, used for water human consumption in Spain, and the Guadiana River, used for irrigation. Human exposure to potentially toxic metals by drinking contaminated water or eating contaminated food can reduce the overall health of the population. Epidemiological studies around the world report the correlation between human diseases and soils contaminated by metals, highlighting the need for remediation strategies to decrease the cost of metals contaminated soils.

The main objective of the INCOME project is to develop a cost-effective data collection and monitoring system, which will contribute to the sustainability management of contaminated regions.

This project aims to characterize the site through the combination of a set of analytical methods and instruments for monitoring contaminated areas, such as biophysical, chemical and geophysical analysis, and hyperspectral remote sensing using sensors onboard of satellites. These tools will allow the optimization and saving of resources in the sampling and analysis stages, providing important information in real-time for decision-making for pollution monitoring and management.

Chemical characterization will consist of the assessment of quality parameters and quantification of potentially toxic metals in soil and water samples as part of the calibration of the proposed model. The great technological innovation of the INCOME project lies in the combination of different methodologies, which are not traditionally combined, for the proposed objective.

This model can be used by several entities that own/manage mines or soils affected by mining activities, for the development of rehabilitation strategies. Risk reduction in contaminated areas is an economically, socially, and environmentally sustainable strategy for the recovery of contaminated soils, especially when the affected areas are extensive.

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P-EnvMonit-29

Co-dispersion of 3,3’,5,5’-tetramethylbenzidine and nanocellulose in water leads to durable iron(III)-responsive suspensions

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Introduction

3,3’,5,5’-tetramethylbenzidine (TMB) is often used in peroxidase-based assays, although it also changes colour when oxidized by certain metal ions [1]. In determinations based on oxidized TMB (ox-TMB), the benzidine turns blue or greenish by the loss of one electron, allowing for naked-eye identification or for quantifications based on measuring the absorbance at 562 nm. Total oxidation, corresponding to the loss of two electrons per TMB molecule, cause yellow coloration with an absorption peak at 452 nm [2]. Frequently, TMB is oxidized by H_2O_2 in the presence of a peroxidase or a so-called “peroxidase mimic”. Few analytes are capable of directly and quickly oxidizing TMB, in absence of peroxidase mimics and in neutral media. This is the case of the iron(III) ion in water [3].

While TMB, in its reduced state, is freely or very soluble in common organic solvents, it is insoluble in neutral aqueous media, unlike ox-TMB. Lowering the pH increases the aqueous solubility of TMB, but at the expense of accelerating its aerial or photo-induced oxidation, losing its chromogenic potential during storage. In practice, TMB is either stored in solid state, within a glass amber bottle and below 8 °C; dissolved in a buffer solution that is kept in the freezer, or dissolved in an aprotic solvent, generally dimethylsulfoxide.

Cellulose nanofibers (CNFs) offer some possibilities to tackle two issues of TMB in aqueous media: insolubility (unless acidified) and chemical instability. The principle is preventing TMB from being solvated by water while it is stably dispersed through an aqueous medium.

Responsive aqueous dispersions of TMB were obtained with anionic CNFs as the only stabilizing agent. A Pickering emulsion approach and the use of a miscible co-solvent were also explored, combining an aqueous CNF suspension with a solution of TMB in either chloroform or ethanol, respectively. The minimum CNF consistency to attain macroscopical homogeneity was 0.18 – 0.30 wt%, depending on the strategy. Both suspensions and emulsions displayed Herschel-Bulkley rheology, with yield stress and with shear-thinning behaviour if the shear stress was high enough.

A chemical stability study was conducted on the three different systems. The co-solvent approach (with ethanol) was the best at protecting TMB under common storage conditions. Moreover, dispersions were used to detect iron(III) ions in water by their optical response: from colourless or whitish to blue (1-electron oxidation). In this regard, emulsions of TMB/chloroform in water outperformed the other systems. After 30 min of reaction, their limit of detection for Fe^{3+} was 1.5 mg L^{-1} (below WHO’s limit for drinking water). Furthermore, TMB dispersions were also apt for paper impregnation and film forming, resulting in visually responsive paper or nanopaper strips. All considered, these systems may offer citizens a decentralized assessment tool to check whether contamination with ferric salts is excessive. Last but not least, although only iron(III) was used in this study as a model analyte, the advantages of nanocellulose stabilization could be extrapolated to other colorimetric systems involving TMB.

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P-EnvMonit-30

PAH Profiles of emitted smoke from burley tobacco stalk briquettes and its combinations with other types of biomass

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Introduction

The current level of agriculture in the world produces a large amount of agricultural waste. In the total share of biomass, the remains of tobacco stalks represent a significant share, given that there are 3.4 million hectares of tobacco worldwide. As making mixtures of tobacco stalks with other types of biomasses (sunflower head remains, wheat straw, corncob, soy straw, and beech sawdust) is not only energetically favourable (1) but also potentially beneficial for the environment, this research aimed to determine whether the combustion of such biomass is environmentally acceptable in terms of the formation of PAH compounds. We made 11 different types of briquettes: six of pure raw materials, including burley tobacco stalks, sunflower head remains, wheat straw, corncob, soy straw, and beech sawdust and five by mixing tobacco stalks with these other raw materials in a 50:50 mass ratio.

All samples were combusted under identical conditions in the same furnace, and sampling was performed on filters. After that, filters were extracted for 32 hours using Soxhlet extraction with dichloromethane as a solvent. Thus obtained extracts were purified by column chromatography. An Agilent GCMS System, 7890A gas chromatograph with HP-5 MS capillary column, was used to identify and quantify PAH compounds. Standard calibration solutions were used to quantify 16 priority PAH compounds from a certified PAH mix solution, AccuStandard, USA, Z-014G-R concentration 1000 ppm.

The highest emission values of PAH compounds in the smoke of tested individual biomasses were obtained by burning briquettes made of corn husks, followed by briquettes composed of remains of sunflower heads and tobacco stalks. Briquettes made of tobacco stalks and corn cobs produced the highest PAH compounds emissions in mixtures. Almost all combinations of tested biomasses with tobacco stalks emitted a smaller amount of PAH compounds than individual biomasses, indicating that combining the tested biomasses is environmentally acceptable and desirable. The reduction of the emission of PAH compounds in mixed briquettes was not observed only in the combination of tobacco stalk - and soybean stem. PAHs with three and four aromatic rings were predominantly formed during combustion, while PAHs with five and six rings were detected to a much lesser extent, usually only in traces. It was observed that combining individual biomasses with tobacco stems in the smoke produced by their combustion decreases the share of aromatic compounds with three rings in all combinations, except for the combination of tobacco stems and remains of sunflower heads.

Our research demonstrates that combining tobacco stem biomass with other types of biomass significantly reduces the emission of harmful PAH compounds during combustion compared to the combustion of individual biomasses. This finding holds great promise for the future of biomass energy production and its potential to mitigate environmental impact.

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P-EnvMonit-31

Canopy density for tree species in an urban park

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Introduction

Forest canopy density is a major factor in evaluating forest status and is an important indicator of possible management interventions. Canopy density refers to the percentage of ground area covered by the overhead canopy of trees or other vegetation. It is a measure of how closely the branches, leaves, and foliage of plants are packed together overhead. Canopy density is important in assessing the microclimate, light availability, and overall ecosystem characteristics of forested or vegetated areas. In this study, we intended to analyse the canopy density of the vegetation for both the coniferous and deciduous tree species within the Pionirski˙ Park. Pionirski Park, with a total area of approximately 3 ha, is located in the narrowest central zone of Belgrade the capital of Serbia. The Park represents the cultural, administrative, and commercial seat and, with its surroundings, occupies an important place in the urban tissue of Belgrade. As part of the entire system of public greenery, Pioneer Park is an important element of the climatic infrastructure. The area of the park consists of three spatially different sub-units. The first one with the highest quality dendrological vegetation. The second unit consists of a flower parterre, and the third part consists of a richly arranged flower parterre with individual trees of tall conifers and deciduous trees. The richness of the park consists of a variety of autochthonous and non-autochthonous dendroflora. The imposing dimensions of the most valuable specimens stand out in particular: English oak (*Quercus robur* L.), European hackberry (*Celtis australis* L.), ginkgo (*Ginkgo biloba* L.), horse chestnut (Aesculus hippocastanum L.). The tree species were determined in the field during the photograph analyses. To obtain the canopy density, hemispherical photographing was used in this study. Field trips have been conducted during August of 2024. Consequently, using the Plant canopy imager C-110 (CID Bio-Science) in total of 71 hemispherical photographs were acquired. Using a self-leveling digital camera, C-110 captures 150° field-of-view images of plant canopies for hemispherical photograph analysis. The imager instantly estimates the Leaf Area Index (LAI) and measures Photosynthetically Active Radiation (PAR) levels. The 24 PAR sensors in the arm of the instrument calculate sunflecks, and measurements can be obtained under any sky condition. The data on the results were evaluated and discussed based on the type of trees and the area of the park in which these canopies were in. The highest value of canopy density of 73.9% was recorded for *Tilia platyphillos*, while the lowest value of 50.4% was recorded for *Cedrus atlantica*. A mean value of 64.4% and a coefficient of variation of 8.23% indicate slight variation in canopy density. The study found that tree species and the different parts of the park do not have a statistically significant influence on canopy density change. Higher canopy density indicates a more continuous, closed canopy, while lower canopy density means the canopy is more open and transparent. Urbane canopy density assessments are foundational to understanding the amount and distribution of tree canopy cover in a community to set goals and targets to strategically increase canopy cover and prioritize the protection of existing tree canopy. Based on the results, it could be concluded that the park is not exposed to major influences that can affect the canopy density. However, our cities often lack the resources to support urban tree canopy assessments as well as efforts to expand, manage and protect urban tree canopy based on the priorities of their individual communities.

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P-EnvMonit-32

Development and improvement of high throughput methods for the determination of emerging pollutants included in the European legislation on water policy

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Introduction

The new proposed legislation on urban wastewater treatment and the water framework directive establish new targets for the removal of pollutants of emerging concern and microplastics in wastewater treatment plants (WWTPs), as well as for the definition of environmental standards [1,2]. Pollutants of emerging concern are a very heterogeneous group of compounds, both in terms of the uses (pharmaceuticals, pesticides, personal care products, plasticisers, industrial reagents, amongst others) and in terms of their properties. It is therefore of great interest to develop analytical methodologies that allow the rapid and simple determination of as many as possible compounds included in these regulations.

In order to respond to these new requirements, the objective of this research was to develop high-performance methodologies that can be used to meet the targets monitoring requirements. In the initial phase of the study, more than 50 organic compounds were selected based on the water directives and proposals for amendments to these directives. Secondly, the methodology for the determination of these compounds was optimised using solid phase extraction (SPE) and liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). Two distinct methodologies based on off-line and on-line SPE were assessed. In the off-line method, good performance was achieved for most of the selected compounds using a sample volume between 100 and 200 mL (depending on the matrix), a 200 mg SPE OASIS HLB cartridge and elution with 10 mL of methanol. Instead, the on-line SPE method, an Agilent Be on-line PLRP-S SPE cartridge, an injection volume of 1.5 mL and elution with acetonitrile were selected. The latter method also worked well for most compounds providing both shorter analysis time and less sample handling, increasing the throughput of the method, however, the limits of quantitation were slightly higher.

Therefore, both optimized methodologies are appropriate to perform targets' monitoring depending on the considered analytes, matrix and therefore, required limits of quantification.

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P-EnvMonit-33

Development of an Enzymatic Biosensor for the Detection of Environmental Stress Markers in Coral Species via Glutathione S-Transferase Reactions

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Introduction

Marine ecosystems are increasingly threatened by a variety of stressors, including shifts in temperature, salinity, pH, as well as anthropogenic pressures such as pollution and overfishing. These stressors can exacerbate oxidative damage in marine organisms, impacting their growth, reproduction, and overall survival. Oxidative stress arises from an imbalance between the production of reactive oxygen species (ROS) and the organism's ability to detoxify them, leading to potentially irreversible cellular damage. Therefore, monitoring biomarkers of oxidative stress is crucial for the effective management and conservation of marine environments. Glutathione, a tripeptide produced by various aquatic organisms, plays a critical role in mitigating oxidative stress by neutralizing ROS and facilitating the detoxification of hydrophobic xenobiotics. Glutathione S-transferase (GST), an enzyme involved in this process, catalyzes the formation of conjugates between glutathione and organic molecules, converting them into more soluble forms that can be expelled by the organisms. Altered glutathione levels in marine organisms can serve as indicators of environmental stress [1].

In this study, we present a novel electrochemical sensor synthesized by alcohol-free sol-gel methodology designed to detect glutathione in seawater based on a GST-mediated reactions. The sensor employs GST to catalyze the reaction between glutathione and p-benzoquinone, an electroactive compound. The reaction forms a glutathione-p-benzoquinone conjugate, which is non-electroactive. The loss of electroactivity of p-benzoquinone in the presence of glutathione is detected through voltammetric measurements. As glutathione concentration increases, the electrochemical response of p-benzoquinone diminishes, indicating the presence and concentration of glutathione.

This approach allows for the sensitive and selective detection of glutathione, providing a powerful tool for assessing oxidative stress markers in marine environments. The development of this biosensor has significant implications for early detection of environmental stress and can enhance the monitoring and conservation efforts in marine ecosystems. By facilitating real-time assessment of oxidative stress levels, this sensor contributes to better understanding and management of the impacts of environmental changes and anthropogenic activities on marine life.

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P-EnvMonit-34

Analytical methodology for the determination of pharmaceuticals and other emerging contaminants used as indicators of the quaternary treatment of urban wastewater

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Introduction

In 2022, the upcoming UWWTD (2022/0345 (COD)) [1] laid down rules on the collection, treatment, and discharge of urban wastewater. The future Directive aims at addressing the environmental and health concerns resulting from the presence of micro-pollutants, other pollutants (*e.g.,* heavy metals, PFAS) and microplastics in European waters. The Directive introduces new treatment processes of wastewater, including quaternary treatment for micro-pollutants.

A minimum percentage of removal of 80 % of six substances used as indicators of the performance of the quaternary treatment is required, out of 13 substances listed in Annex I, and divided in two categories: substances that can be very easily treated and substances that can be very easily disposed of. Many pharmaceuticals are included in this list, such as venlafaxine, carbamazepine, citalopram, diclofenac, clarithromycin, candesartan and irbesartan.

The aim of this work is the development of a new analytical methodology to determine the above-mentioned pharmaceuticals and other emerging contaminants in wastewater samples. The method is based on solid-phase extraction (SPE) followed by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) and by ultra-high performance liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (LC-QTOF-HRMS). Several parameters that may influence the extraction are optimized including type of sorbent and cartridge, sample volume and pH, elution volume and breakthrough volume. The methodology will be validated in terms of analytical figures, and applied to wastewater, including samples collected after sludge centrifugation from anaerobic digestion (centrate) and after tertiary treatment using a Membrane Bioreactor (MBR).

The comparison between cartridge sorbent and sample pH shows better recoveries with the use of a polymeric reverse phase and acidic conditions. Almost all substances listed in Annex I, such as carbamazepine, citalopram, diclofenac, venlafaxine, benzotriazole, candesartan or irbesartan, are detected in the centrate.

These first results are promising and should help assess the risks that the discharge of the targeted contaminants in urban wastewater poses on the environment and public health.

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P-EnvMonit-35

Assessment of the level of self-cleaning of the soils around the former metallurgical plant – Kremikovtsi, Bulgaria

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Introduction

The present research aims to study the natural self-cleaning ability of soils around the metallurgical plant – Kremikovtsi, Bulgaria closed since 2009. On the basis of results from previous survey [1] with soil samples collected nearby the operating Kremikovtsi plant, we had prepared a new sampling plan including sample points of contaminated soils according to the current Bulgarian soil legislation [2]. The new set of samples was collected, processed, and analyzed following internationally accepted ISO standards for soils [3-5] in 2017, eight years after closing the plant. Encouraged by the optimistic results, we collected new soil samples from the 2017 sampling points set to check the remediation processes 14 years (2023) after closing the Kremikovtsi metallurgical plant, following internationally accepted ISO standards for soils [5-9]. Appropriate analytical techniques (FAAS/ETAAS) were used for the quantification of both pseudo-total concentrations and concentrations of selected toxic elements in soil extracts, obtained according to the classical BCR extraction. The content of polycyclic aromatic hydrocarbons (PAHs) in soil samples was determined by gas chromatography, after a Soxhlet extraction.
Comparing the data from the previous studies and the newly obtained results, self-purification coefficients for the sampling points were calculated with respect to the different analytes (toxic chemical elements and PAHs).

Acknowledgements

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P-EnvMonit-36

The presence of plastic pollution in the biosphere reserve of the Tara River Basin

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Introduction

Due to the increased production of plastic materials, their long life span, short period of use of plastic products there is an increased amount of plastic waste in the world [1]. According to the size, plastics are classified into: megaplastics, macroplastics, mesoplastics, microplastics and nanoplastics [2]. Most plastics in the environment end up in aquatic ecosystems [3]. Rivers are considered the main transportation routes of plastics of various sizes, while river sediment are considered the "final precipitator" of plastic in aquatic ecosystems [4]. The objective of the present study is to determine plastic abundance and identification in surface sediment of biosphere reserve of the Tara River Basin.

Tara is the most beautiful, clearest and longest river that flows through Montenegro. The length of the Tara River is 157 km, and the basin area is 1853 km². Tara River has been under UNESCO protection since 1977 as part of the "Man and Biosphere" (MAB) program. Due to the great importance of the Tara River, as well as the possible negative anthropogenic impact on the river, this study examined the presence of plastics in selected localities along the river course. Surface coastal sediments of Tara river were collected at 15 selected locations. For density separation was used concentrated NaCl solution. Samples were visual analyzed under a microscope, while their chemical structure was analyzed using ATR-FTIR spectroscopy.

Plastic different sizes were identified at all selected locations of coastal sediment of the Tara River with varying degree of concentration (50–590 plastic items/kg of dry sediment). The results indicate that sediments of Tara River in the present study are moderately polluted with plastic compared with literature data. In coastal sediment of the Tara River the primary plastic shape types by number were fibers and fragments, blue, clear and red in color. The most abundant polymer types in the coastal sediment of the Tara River were polyethylene and polypropylene.

Population density, wastewater discharge, inadequate solid waste management, tourist and fishing activities were identified as the main sources of plastic pollution in Tara River in Montenegro. The identifcation of the plastic pollution in Tara River may allow the decision-makers to consider how to reduce plastic-derived pollution in order to maintain and preserve this valuable natural reserve protected by UNESCO in the best way.

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P-EnvMonit-37

Methods for fluorine determination in raw material for gasoline blending

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Introduction

Gasoline, the most valuable product of a crude oil refinery, is obtained in a blending process where more than 120 hydrocarbon streams can be used [1]. The most important raw materials come from catalytic processes such as reforming, cracking, hydrocracking, isomerization and alkylation. Some catalysts can contain fluorine compounds or can be activated by them [1]. Especially in the alkylation process, concentrated hydrofluoric acid is used as a catalyst. If the installation does not operate properly, side products, such as organic fluorides (FO), can be formed. More than 150 mg L^{-1} of fluorine was detected in alkalyte [2]. The presence of FO in gasoline is harmful due to the direct pollution of the environment as well as intensive corrosion caused by the HF released in the decomposition of FO. Unfortunately, determining fluorine in gasoline is not obligatory and is performed very rarely. The aim of this presentation is to discuss and compare analytical methods that have been applied for fluorine determination in raw materials for gasoline blending. The popular and most important analytical techniques used for fluorine determination in a variety of materials are potentiometry with fluoride ion selective electrode (ISE) and ion chromatography (IC) [1,3]. Both methods need sample decomposition and fluorine transformation into fluoride anion. Due to the high energy of the C-F bond (552 kJ mol^{-1}), aggressive decomposition methods have to be applied, for example, reaction with sodium biphenyl, pyrohydrolysis or combustion in oxyhydrogen flame in a Wickbold's apparatus. Combustion in pyrohydrolysis conditions is also applied in the combustion ion chromatography variant [4]. Generally, the need for sample decomposition increases analysis time and uncertainty (the dangers of analyte losses, contamination, deteriorated and variable combustion efficiency for various fluorine compounds) and creates environmental hazards. The new alternative for fluorine determination is high-resolution continuum source flame molecular absorption spectrometry (HR-CS FMAS) [1,2,5]. The method relies on measuring the absorption of radiation of a high-intensity xenon lamp by monofluorides, which are purposely synthesized in an air-acetylene flame. Gallium [1], calcium [5] and strontium [2] monofluorides have been applied as the target molecules. The measured absorption is related to the rotations of the molecules. The radiation is isolated using a double monochromator (comprising a prism and an echelle grating) and detected using a linear charge-coupled devise array detector. The methods of fluorine determination using HR-CS FMAS are fast and comfortable, as gasoline samples do not need to be decomposed (samples are only diluted in xylene). The best method detection limit, 1 mg L^{-1}, has been obtained with SrF as the target molecule [3], which was achieved, among others, due to the better solubility of the used organic Sr salt and the summing of signals of many pixels. In order to improve detectability further, the flame was substituted with a graphite furnace. Although the high-resolution continuum source graphite furnace molecular absorption spectrometry (HR-CS GFMAS) technique is widely applied for fluorine determination and enables the detection of 5 pg of fluorine [6-7], its application for fluorine determination in gasoline turned out to be a great challenge. The organic fluorine compounds present in gasoline components and these used as standards are volatile; despite many efforts, immediate evaporation and losses of volatile OF from the graphite furnace took place. Finally, some promising results have been obtained using HR-CS GFMAS and CaF as the target molecule with calcium-containing oil as the source of calcium. In the presentation, both the disadvantages and advantages of various ways of fluorine determination in raw materials for gasoline blending will be discussed and critically compared. Special attention will be paid to the accuracy of the analysis.

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P-EnvMonit-38

Field validation of a novel passive air sampler – monitoring of semivolatile organic pollutants in the remote marine and continental boundary layer

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Introduction

Passive air sampling (PAS) of trace organic substances in ambient air is cost-efficient and allows access to sites without infrastructure, but well-defined sampling of the particulate phase and too low time resolution remain a challenge. [1]

The Venturi Experiment MPI (VEMPI) sampler is constructed of a bundle of 10 conical Venturi tubes. The annular gaps of the tubes are interconnected and join into a collection tube connected to gas (4 PUF plugs in series) and particulate phase (2 parallel 47 mm glass fibre filters) sampling media. VEMPI was validated by side-by-side sampling with active air samplers at a central European continental site (Košetice, 49°34′N/15°05′E, 520 m a.s.l.) and a Caribbean coastal site (Deebles Point, Barbados, 13.16°'N/59.40°W, 12 m a.s.l.).

Following Soxhlet extraction (DCM) and clean-up, 26 polycyclic aromatic hydrocarbons (PAHs), 9 polychlorinated biphenyls (PCBs) and 32 organochlorine pesticides (OCPs, including derivatives thereof) were analysed using GC (7890A or 8890A Agilent) coupled to triple-quadrupole MS (7000B or 7000D, Agilent), while for 19 nitro- and 12 oxygenated PAHs (NPAHs, OPAHs), the GC was coupled to an APCI-MS/MS (Xevo TQ-S, Waters).

Sample air flow rates ranged 1-13 $m^3\ d^{-1}$ depending on wind velocity. The sampler is found suitable for monitoring OCPs and PCBs in mostly the 0.1-1 $pg\ m^{-3}$ concentration range). For some OCPs, heptachlor and chlordane, these levels are among the lowest concentrations in air ever reported. In the continental boundary layer, at a rural site, vertical distributions indicate the dominance of advection over local emissions for most substances in all seasons, unlike previously reported from urban sites. Indications for local sources (ctot 230m/ctot 3m <1) are seasonally found for triphenylene, retene, dibenzofuran, 2-nitronaphthalene and 2-nitrofluoranthene, which is possibly related to re-volatilisation.

Because of the blow-off sampling artefact, the VEMPI sampler cannot differentiate between gas and particulate phases, but collects $c_{tot} = c_g + c_p$ artefact-free.

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PY-EnvMonit-01

Use of ceramic passive samplers as an alternative for monitoring contaminants of emerging concern in groundwater

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Introduction

Assessing water quality is becoming increasingly critical due to the growing threats to water availability posed by global warming and ecological changes. The European Union estimates that 26% of groundwater bodies do not achieve good chemical status [1]. One of the main steps to allow an accurate evaluation of the chemical quality of water is the sampling methodology. Traditional methods for sampling groundwater, such as grab sampling and autosampler devices, have limitations offering only a snapshot of contamination levels at the time of collection. These methods are susceptible to fluctuations in contaminant concentrations, requiring repeated sampling to capture an accurate picture of the pollution status over time. Consequently, alternative sampling methods that provide more representative or averaged contamination levels hold great promise.

Ceramic passive samplers (CPSs) consist of a porous ceramic cylinder that allow the diffusion of contaminants to the inner part which are thereafter retained in a sorbent material. They can be deployed for extended periods of time, ranging from weeks to months [2][3]. Upon retrieval of the CPS, the analytes are extracted and quantified using liquid chromatography-mass spectrometry (HPLC-MS). The result is expressed as the absolute mass of each analyte, reflecting the total amount accumulated during the deployment period.

In this study, we measured the concentration of several Contaminants of Emerging Concern (CEC) using both CPS and grab sampling methods in wells located in the Besós catchment area in Barcelona, Spain. The comparison showed that passive sampling effectively concentrated contaminants by several orders of magnitude, increasing sensitivity and yielding concentrations that, for many compounds, were of the same order of magnitude as those found through grab sampling. We have observed that pharmaceuticals such as acetaminophen, metformin, venlafaxine and valsartan were detected at concentrations mostly in the 0.1-200 ng/L range, and their main pollution source as leaking from the sewage system. Other contaminants detected were artificial sweeteners such as saccharin and acesulfame, which are excreted after human consumption and may originate from the sewage system too. Overall, we have observed that groundwaters from the Besos river are affected by a myriad or organic contaminants, and we highlight the need for the long-term monitoring to protect this important water resource.

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PY-EnvMonit-02

New magnetic sorbent for trace metal analysis in wastewater samples

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Introduction

Environmental pollution resulting from industrial processes and human activities is one of the most pressing issues today [1]. In particular, heavy metal contamination has significantly increased in recent years, becoming a major concern for environmental agencies worldwide. Some trace metals can enter the human body, leading to various health problems [2]. Therefore, the detection of these hazardous metals in water and aquatic ecosystems is of great importance. To address this, a simple, sensitive, and matrix effect-free analytical method has been developed for the simultaneous determination of Ba, Be, Cd, Cr, Cu, Fe, Hg, Mn, Ni, Pb, and Zn in wastewater samples using inductively coupled plasma optical emission spectrometry (ICP OES). To enhance the method sensitivity, magnetic dispersive solid phase extraction (MDSPE) was employed, utilizing a new magnetic carbon material (zeolitic imidazolate frameworks), which offers high chemical stability, large surface area, and porosity. This material consists of tetrahedrally-coordinated transition metals (such as cobalt) linked by imidazolate ligands. Additionally, the key experimental factors influencing the MDSPE procedure were optimized using multivariate analysis. Under optimal conditions, sensitivity, repeatability, limits of detection and quantification were determined. Trueness was also evaluated through recovery experiments in a real wastewater sample and by analyzing a certified reference material.

Acknowledgements

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PY-EnvMonit-03

Standardization of microwave-assisted extraction procedures for characterizing metallic nanoparticles in environmental samples by means single particle ICP-MS

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Introduction

Nanomaterials (NMs) present in environmental sample are usually characterized by means single particle inductively coupled plasma mass spectrometry (spICP-MS) after an extraction treatment. To this end, different sample preparation strategies (e.g., liquid extraction at ambient temperature, ultrasound-assisted extraction, etc.) have been proposed in the literature but they do not always provide accurate results and show a limited sample throughput. Recently, our research group has recently demonstrated the benefits of using microwave-assisted extraction (MAE) treatments for extracting NMs from soils and air filter samples [1-2]. For instance, Au- and PtNPs were quantitatively recovered by treating samples with 20mL of a 0.1 M NaOH solution in a 800 W domestic microwave oven (DMO) for 6 minutes. Though the use of MAE overcomes main drawbacks shown by previous strategies, the use of DMO entails significant practical disadvantages (e.g., lack of sample heating control, poor reproducibility due to solution splashes, etc.). The aim of this work is to adapt previously developed MAE treatments with DMOs to state-of-the-art scientific microwave oven digestion systems (SMO). Thus, MAE treatments can be standardized for routine analysis and improve spICP-MS metrology. By the appropriate optimization of operating conditions, metallic NMs can be efficiently isolated from soils and air samples using a MW power of 1200 W and 10mL of NaOH 0.1M solution in 10 and 6 min, respectively. When compared to DMO, the use of SMO provided better accuracy, precision, and sample throughput (6-fold).

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PY-EnvMonit-04

Biomonitoring of metals in the urine of children from the Valencian Region (Spain): Levels, predictors of exposure, and risk assessment

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Introduction

We are exposed to metals since they are an inherent component of the environment, but some of them are also classified as priority hazardous substances.[1] Children are a vulnerable group because, compared to adults, they may be exposed to greater levels of metals resulting from their larger intake of food and drink relative to body weight. [2] The present study analysed the levels of 20 metals in the urine of 604 children aged 6 to 11 years in the Valencia region of Spain, together with socio-demographic and dietary associated factors. The focus was on seven essential metals (Co, Cu, Mn, Mo, Se, Zn and V) and 13 toxic metals (Al, Sb, As, Ba, Be, Cd, Cs, Pb, Ni, Pt, Th, Tl and U). The urine sample was diluted 1/10 with deionised water and 100 µL of HNO_3 and chemical analyses were performed on ICP-MS (iCAP RQ Thermo Scientific and Nexion 300-x Perkin Elmer). Risk assessments were performed for three essential metals (Se, Mo, Zn) and five toxic metals (Al, Ba, Cd, iAs, Tl) based on established benchmarks. All essential metals except Co (91%), Mn (73%) and V (97%) showed 100% detection frequencies, with geometric mean (GM) concentrations ranging from 0.09 µg/L (Mn) to 49 µg/L (Mo) (Zn was 389 µg/L). For toxic metals, Ni, As, Cs, Ba, Tl, Pb had detection frequencies between 98-100%, with GM concentrations between 0.16 µg/L (Tl) and 33 µg/L (As). Urinary metal concentrations were predicted using sociodemographic and dietary factors. The age of the children was positive correlated with Be and negatively correlated with the amounts of Al, Cs, Co, Cu, Mo, Se, Tl, and Zn. Children with foreign parents had greater amounts of Al, whereas children born foreign had lower quantities of Be and As. The concentrations of As, Be, and Se were positive correlated with fish consumption. Besides that, a higher intakes of meat products leads to an increase in concentrations of Pb but a decrease in concentrations of Al. Hazard quotients (HQ) for As and Al were found to be more than 1, according to the risk assessment. This suggests that these metals require priority risk assessment or management follow-up.

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PY-EnvMonit-05

The ageing process of peloids from Koviljača Spa (Serbia)

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Introduction

Peloid or healing mud represents maturated mud or muddy dispersion with healing and/or cosmetic properties, composed of a complex mixture of fine-grained natural materials of geological and/or biological origin and mineral water. Solid and liquid phases mix and interact within the ageing or maturation process, accompanied by biological activity. In this process, the alteration of both the organic and inorganic characteristics of peloids occurs. These processes improve the final quality of peloids, implying changes in physicochemical properties, such as improved cooling kinetics, plasticity, viscosity and hydration capacity [1, 2].

There are several peloid-rich areas in Serbia, and many of them are formed as well-known spas. Koviljača spa is one of the most popular in western Serbia, on the right bank of the Drina. It is known for its rich sulphurous water springs (rich in hydrogen sulfide), sulphur mud/peloid, and favourable climatic conditions. In Koviljača Spa, peloid is formed from soil with a high percentage of clay placed in special pools troughs with a constant inflow of sulphur water, where it is occasionally mixed and usually matures for 2-3 years. In these pools, the mud is additionally "enriched" with specific grass and algae, which gives a characteristic dark green colour. After maturation, the mud is dried and introduced into the therapeutic area, while after application, it is recycled by returning to the pools. This study aimed to follow the distribution of saturated and aromatic hydrocarbons to define the optimal time for the maturation of the peloid.

Samples of peloid from Koviljača spa are taken from different pools where the mud stayed for 2 years, 1 year, and 6 months, as well as samples of the initial soil (before mixing with termomineral water) and of mud which stayed right below the spring of this thermomineral sulfur water. The samples were dried and ground before analysis. Organic matter was extracted by Soxhlet extraction. Organic extracts are separated by column chromatography into saturated and aromatic hydrocarbons. The fractions were analysed by GC-MS [2].

The distribution of saturated hydrocarbons is dominated by diterpanes (16α(H)-phyllocladane and pimarane) and odd long-chained *n*-alkanes (n-C_{27}, n-C_{29}, n-C_{31}) with the maximum at n-C_{31} in the most mature peloid sample which stay in pool 2 years. Such distribution results from the origin of organic matter rather than maturation processes. The high contents of n-C_{27}, n-C_{29}, and n-C_{31} alkanes indicate a significant contribution of epicuticular waxes since phyllocladane-type diterpenoids refer to the peloid-forming plants belonging to the conifer families. Aromatic hydrocarbons detected in the most mature peloid sample characterise the prevalence of long-chain methyl esters of carboxylic acids.

The maturation process can prompt the development of specific harmless and nonpathogenic microbial communities, which contribute to the formation of therapeutically active compounds during their metabolic activity/degradation, thus enhancing the healing benefits of peloids [1]. Also, some factors that affect the maturation process are adhesion, rheology, grain size distribution, microfabric, cationic exchange capacity, crystallinity etc. In addition, the distribution of lipid biomarkers is associated with terrestrial precursor biomass. Thus, the prevalence of long-chain *n*-alkanes and methyl esters of carboxylic acids contributes to thermotherapeutic and anti-inflammatory effects of peloids.

Acknowledgements

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PY-EnvMonit-06

Rapid analyis of chromium species by µLC-ICP-MS

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Introduction

Chromium (Cr) is a transitional element with oxidation states spanning from -2 to +6. The prevalent stable forms of chromium found in the environment are trivalent Cr(III) and hexavalent Cr(VI) compounds. Cr(III) serves as a vital micronutrient for human health, whereas Cr(VI) is notorious for its high toxicity and carcinogenic properties. Separating these two chromium species is crucial due to their disparate toxicities, but separating both species poses a significant challenge as they exhibit instability under varying conditions of temperature and pH. Cr(III) is stable in acidic conditions and Cr(VI) in alkaline conditions. Therefore, interconversions between Cr species may occur in complex matrices like biological fluids and during analysis, hence making their accurate determination very difficult. Moreover, both Cr species are frequently found in low concentrations. Therefore, an improved sensitive and robust method for the simultaneous determination of Cr(III) and Cr(VI) in biological fluids, such as exhaled breath condensate, urine, waste water and nutrition solution, has been developed.

The method uses a hyphenated micro liquid chromatography (µLC) system coupled to inductively coupled plasma mass spectrometry (ICP-MS). The optimised method incorporates a pH adjusted EDTA complexation step to stabilise Cr(VI) and Cr(III). The µLC system uses an anion exchange micro-sized column to separate the Cr species.

Cr(III) and Cr(VI) were separated with different retention times at 170 and 230 sec, respectively. The method was optimized and validated by spiking Cr(III) and Cr(VI) in various samples of biological fluids. Furthermore, the method was validated using a drinking water proficiency testing material sample.

The developed method can be used for rapid routine determination of chromium species with high precision and reliability.

PY-EnvMonit-07

Electroanalytical sensing of nitrates in cyanobacteria growth media at electrified liquid-liquid interface

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Introduction

The polarized liquid-liquid interface also known as the interface between two immiscible electrolyte solutions (ITIES) is commonly used to study the transfer of charged molecules between two liquid phases that do not mix. The difference in electrochemical potential of the two contacted phases creates an electrical potential drop, which can be harvested to power various chemical and physical processes such as interfacial ion transfer and adsorption. ITIES can be used to study chemical molecules that can not be easily oxidized/reduced with traditional three-electrode-based electrochemical systems [1,2].

Excessive nitrate levels in the biosphere pose significant risks to plant and human health, despite their essential role, especially for plant growth and functioning. In our study, we have developed an innovative method for onsite periodic monitoring of nitrate concentrations in cyanobacteria growth media using an electrified liquid-liquid interface (eLLI) and voltammetry. This approach allows for real-time monitoring of nitrates, with the detection signal directly linked to NO_3^- transfer across the liquid-liquid interface. The ion transfer voltammograms recorded at the eLLI system provided key analytical parameters, including a linear detection range of 20 to 500 μM and detection and quantification limits of 1.5 and 14.6 μM, respectively. We have also developed a simple methodology to eliminate the interfering effect of abundant Cl^-.

Our results demonstrate that the eLLI-based nitrate sensor delivers exceptional analytical performance for measuring nitrate levels in Z8 cyanobacteria growth media medium, which contains nitrates and several dozen additional nutrients (the electrochemical behavior of each was investigated at the eLLI). The sensor was also successful in the periodic monitoring of nitrate levels in *Microcystis Aeruginosa* cyanobacteria samples cultured in Z8 medium. During this presentation, I will provide a detailed discussion on the methodology, its advantages, and the practical outcomes achieved [3].

Acknowledgements

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PY-EnvMonit-08

Occurrence and potential sources of Polycyclic Aromatic Hydrocarbons (PAHs) in Red River sediments, from Hanoi to the rivermouth (Vietnam)

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Introduction

Rapid growth of urbanization and industrialization contributes significantly to the occurrence of contaminants in the environment. Vietnam, a developing country in Southeast Asia, has witnessed a fast rate of industrialization, contributing significantly to the rapid development of the nation's economy. One of the most important economic regions of Vietnam is the Red River Delta (e.g. aquaculture, agriculture, textile and light industries). The Red River also plays a vital role as an essential freshwater source and waterways for transportation. Hence, the river is under strong anthropogenic influence and highly susceptible to contamination by persistent and ubiquitin micropollutants, such as polycyclic aromatic hydrocarbons (PAHs). But the quality status of this geographical area is still scarcely documented.

PAHs are a group of organic substances containing fused benzene rings which are the products of the incomplete combustion or pyrolysis of organic matter. Based on their origins, PAHs can be classified into two main groups: petrogenic (derived from petroleum products) and pyrogenic (incomplete combustion processes) [1]. Being carcinogenic and endocrine disrupting, 16 PAHs had been designated as priority pollutants by the United States Environmental Protection Agency (EPA) since 1976.

The aim of this study is to i) analyze the occurrence of the 16 US EPA priority PAHs in sediment samples collected from 3 sampling campaigns during the dry (March 2023) and rainy seasons (June and September 2023), ii) identify their potential sources and iii) assess the potential environmental risk. The sediment samples were extracted by Accelerated Solvent Extractor (ASE 200, Thermo Scientific™ Dionex) and analyzed by gas chromatography coupled with mass spectrometry (GC–MS; Autosystem XL GC and TurboMassTM, Perkin Elmer).

PAH concentrations ranged from 17 to 109 ng.g^{-1}, dry weight (dw). PAHs levels in the Red River sediment samples collected in 3 sampling campaigns were well below the Vietnam's national standards for freshwater sediment and significantly lower than those of other urban rivers in Vietnam [2]. The total organic carbon (TOC) content of sediments showed positive linear correlation with PAH concentrations ($p<0.01$, Pearson's Correlation test). Therefore, low TOC content (0.19-1.23%) could explain for the low contamination level of PAHs in sediment samples. While there was no obvious upstream-downstream trend, the t-test revealed that the PAH levels were significantly higher ($p < 0.05$) in the middle of rainy season than in the late dry season. The distribution of PAHs congeners was consistent throughout the studied periods and followed the order: 4 > 5 > 3 > 6 > 2-ring. Diagnostic ratios indicated a pyrogenic origin of PAHs, coming from the biomass and fossil fuels combustion. According to risk assessment, it can be inferred that the presence of PAHs in sediments of the Red River is only rarely expected to have effects on humans and living organisms.

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PY-EnvMonit-09

In-vivo bioavailability of bisphenol A associated to microplastics. Are plastic particles “bioavailability vectors”?

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Introduction

This work aims at determining the bioavailability of BPA adsorbed onto microplastics (PE-BPA) when ingested orally by rats, and to compare it against the bioavailability of dissolved BPA in the gastrointestinal tract. To this end, two groups of n=6 adult Wistar rats (3 females and 3 males) were orally administered with 0.67 mg BPA/kg rat with either free BPA dissolved in corn oil or BPA adsorbed onto PE microplastics with average dimensions of about 100 μm dispersed in carboxymethylcellulose (CMC). Moreover, for quality control and accuracy, two control groups were included in the study, one containing the CMC and the oil vehicle (Control CMC-oil), and another containing the vehicle and microplastic blank (Control PE). Plasma samples were collected at Time A= 0h, 0.5h, 2h, and 6h from three rats in each group (2 males and 1 female), and at time B= 0h, 1h, 4h, and 24h from the remaining three rats (2 females and 1 male) post-administration. Purification and detection of both the principal BPA metabolite in plasma, that is, the conjugate BPA-glucuronide (BPAg), and the parent compound were performed using solid-phase extraction with Captiva EMR-Lipid (40 mg). Quantification of the analytes was accomplished by an LC-MS system. Separations were performed on a C18-Luna column (150 × 2.1 mm). Bisphenol A-d_{16} and BPAg-$^{13}C_{12}$ were used as internal standards.

The toxicokinetic profiles of both BPA and BPAg showed a maximum absorption peak at the T_{max} indicated in Table 1, followed by a gradual decrease up to 24 h but they did not reach the basal level yet. The area under the plasmatic concentration-time curve (AUC) was used to assess and quantify the overall exposure of rats to BPA and PE-BPA. Due to the low concentrations of BPA found, resulting from its metabolism to BPAg, the statistical analysis was conducted using the AUC values of only BPAg for each treatment group. Both $AUC_{0\text{-}6h}$ and $AUC_{0\text{-}24h}$ values of PE-BPA groups showed no significant differences ($p\text{-value} > 0.05$) compared to the BPA group (Table 1), indicating that the bioavailability of free BPA compared to BPA adhered to microplastics is not statistically different. Moreover, a preliminary study on bioavailability based on sex was conducted with the experimental data by generating two kinetic curves per sex, combining values from Time A and Time B. The $AUC_{0\text{-}24h}$ values showed no statistically significant differences between sexes ($p\text{-values} > 0.05$) in either the BPA or PE-BPA groups, likely due to the small sample sizes. However, a trend toward higher plasma concentrations of BPAg was observed in males, with $AUC_{0\text{-}24h}$ values of 4789 ± 2443 for the BPA group and 6412 ± 738 for the PE-BPA group, compared to 1910 ± 280 and 4009 ± 509 for females, respectively.

		Control CMC-oil	Control PE	BPA	PE-BPA
BP Ag	T_{max}(h)*	1.5±2.2	2.6±2.4	2.7±2.3	4.3±1.5
	C_{max}(μg/L)	10.9±8.2	7.8±5.8	216±120	341±122
	$AUC_{0\rightarrow6h}$(μg h/L)	96±28	39±10	1344±428	1608±139
	$AUC_{0\rightarrow24h}$(μg h/L)	32±11	60±12	2325±634	3586±526
BP A	T_{max}(h)*	1.8±1.3	3.4±2.6	2.4±2.6	2.9±2.8
	C_{max}(μg/L)	5.7±1.8	4.3±1.5	8.3±6.4	6.8±1.9
	$AUC_{0\rightarrow6h}$(μg h/L)	22±1	33±6	48±17	29±3
	$AUC_{0\rightarrow24h}$(μg h/L)	64±9	74±16	106±14	99±8

Table 1. Toxicokinetic parameters of BPAg and BPA in rats after the oral administration of BPA and PE-BPA.
**Calculated based on discrete data t= 0, 0.5, 1, 2, 4, 6, 24 h.*

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PY-EnvMonit-10

Smartphone-based fluorescence imaging system for rapid detection of microplastics in urban stormwater

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Introduction

Microplastics, synthetic polymers with particle sizes ranging from 1 µm to 5000 µm, have become a pressing global issue[1]. As of 2015, out of the over 6.3 billion metric tonnes of plastic waste produced globally, only 9% was recycled, 12% was incinerated, and 79% ended up in landfills or the natural environment[2].

Urban stormwater runoff is a significant carrier of microplastic contamination into freshwater and marine environments, where microplastics are a threat to ecosystems and human health[3]. A rapid and effective on-site screening method for detecting and measuring microplastics in urban stormwater runoff is thus essential to help understand the sources and mechanisms of microplastic pollution in urban environments.

This work presents a portable fluorescence imaging system for on-site analysis of stained microplastics consisting of an enclosed 3D-printed case, equipped with a blue light-emitting source and an orange filter to block blue light, and smartphone detection. The case was fabricated with black PLA material using a Raise Pro 3D printer. Water runoff samples collected in urban areas of Dublin were subjected to organic matter digestion, density separation to remove inorganic matter and size fractionation. Four solvents were evaluated for their effectiveness in staining microplastics without degradation. The microplastic particles were stained directly on the filter and in solution. Images were then taken of the entire membrane filter area with a smartphone camera. This fluorescence imaging system offers a user-friendly, simple, and portable alternative to traditional microscopy for analysing microplastics in water runoff samples, making it easier to monitor microplastic pollution in urban environments.

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PY-EnvMonit-11

Diatom-derived extracellular polymeric substances affect silver nanoparticles fate in freshwater via eco-corona formation

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Introduction

Silver nanoparticles (nAg) are widely used in various fields and are frequently released into aquatic environments, where their behavior is influenced by environmental conditions. One significant yet underexplored factor affecting the fate of nAg in these environments is the role of extracellular polymeric substances (EPS) released from aquatic phytoplankton [1].This study investigates the interactions between EPS from the diatom *Cyclotella meneghiniana* and 20 nm citrate-coated nAg, focusing on how do EPS influence the surface properties, colloidal stability, and dissolution of nAg in freshwater settings [2].

Using a combination of advanced spectroscopic and imaging techniques, the study explores the behavior of nAg when incubated with EPS isolated from an axenic *C. meneghiniana* culture. The interaction was studied over both short-term (2 h) and long-term (72 h) periods in a simulated synthetic freshwater environment. Moreover, four different concentrations of EPS were tested to assess a possible concentration dependent effect on the transformations of nAg.

The analyses revealed that the EPS produced by *C. meneghiniana* are rich in polysaccharides and proteins, which can affect the transformations and behavior of nanoparticles [2]. The results show that the EPS enhanced the colloidal stability of the silver nanoparticles by adsorbing onto their surface and inducing steric repulsion, with consequent prevention of aggregation process otherwise occurred in the medium in absence of EPS. In addition, EPS hinder homo-aggregation, also through Ostwald ripening phenomenon, in the absence of EPS but promoted less strong hetero-aggregation processes with a concentration dependent effect: higher EPS concentrations corresponded to higher sized hetero-aggregates. EPS, in fact, worked at the same time as a hindering agent of homo aggregation processes linked to ionic strength of the medium and as a promoter of hetero aggregated formation through bridging effect of adsorbed EPS. Moreover, the EPS, through the eco-corona formation, decreased nAg dissolution, reducing the release of silver ions, which are primarily responsible for the toxicity of nAg [1].

Transmission electron microscopy (TEM) images assessed, through negative staining with uranyl acetate, the formation of an eco-corona on the nAg surface attributed to the diverse components within the EPS, showing the bridging effect of EPS. Evaluation of the main components adsorbed on nAg demonstrated that both polysaccharides and proteins were involved. Higher percentage of proteins was adsorbed on nAg over time in comparison with polysaccharides, showing higher affinity of protein fraction to nAg. Protein stronger involvement in ecocorona formation was demonstrated by fluorescence quenching confirming the formation of EPS-nAg complex through hydrophobic interactions with nAg.

The results of the present study suggest that by enhancing colloidal stability and reducing dissolution rates, the EPS could significantly influence the environmental fate and potential ecological risks of nAg in EPS-abundant waters.

Acknowledgements

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PY-EnvMonit-12

Contrasting level of contaminants in different urban land uses depending on the identity

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Introduction

Nowadays, the uncontrolled use of chemical products such as pesticides, as well as the poor management of waste, mainly plastics, has significantly contributed to increased environmental pollution. Studies on environmental pollution in urban areas are scarce, and are comparison with nearby natural areas are uncommon, despite the expectation that urban areas would be much more polluted. Urban areas have a great variety of land uses with different managements, which can affect their levels of different contaminants. This study assesses the contamination of four different urban green spaces across the Iberian Peninsula and compared them with natural areas nearby. Soil samples were collected from 54 cities and included five land use categories: Natural or Semi-natural Ecosystems, Urban Parks, Urban Crops, Golf Courses and Green Roundabouts.

Four types of soil contaminants, namely metals, pesticides, microplastics and dumps were studied. Metals (Cu, Pb, Cd, Zn, Ni, Cr, As) were determined and quantified by inductively coupled plasma optical emission spectrometry (ICP-OES); pesticides were determined by high-performance liquid chromatography coupled to tandem mass spectrometry (UHPLC-MS) focusing on 16 different pesticides; microplastics were extracted by density separation after pre-treatment with Fenton's reagent and determined by laser direct infrared microscopy (LDIR). The rubbish present in the different urban spaces was quantified and classified to determine the direct contamination derived from human activity. Regarding metals, the natural area and the golf course had a lower concentration of metals than the rest of the urban areas, with Zn being the most abundant metal in all the green spaces studied. In relation to pesticides, their concentration was lower in the natural area than in the urban areas, being notably higher in golf courses and urban crops. The fungicide family had the highest concentrations among pesticides with boscalid being the most abundant fungicide. In contrast to the other pollutants, microplastics were more prevalent in the natural areas. The highest concentration of microplastics corresponded to fragments and films dominated by polymers such as polyethylene terephthalate (PET) and polyurethane (PU). The abundance of rubbish was higher in urban than in natural areas, except for the golf courses, which were the least polluted with dumps, with plastics representing the largest fraction of waste in all areas. In general, excluding microplastics, all pollutants predominated in urban areas with respect to natural areas, but the type of land use of the urban area influenced the levels of different contaminants.

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PY-EnvMonit-13

Biodegradable vs. fossil-based mulch: Sorption study of azoxystrobin on pristine and aged particles

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Introduction

Plastic mulch is extensively utilized in agriculture for its benefits in retaining soil moisture and temperature, preventing weed growth, reducing soil erosion, and enhancing crop yields [1]. However, it is a significant source of microplastics (MPs) in agricultural soils, second only to air deposition. The accumulation of plastic mulch in soil has raised concerns due to its adverse effects on soil structure, crop growth, soil enzyme activity, and microbial diversity [2,3]. Traditionally, mulch is made from fossil-based polymers such as polyamide, polyethylene (PE), polystyrene, and polyvinyl chloride. Since the 1980s, biodegradable polymers like polylactic acid (PLA), polybutylene adipate terephthalate (PBAT), and polybutylene succinate (PBS) have been introduced [4]. These biodegradable mulches degrade completely only under optimized composting conditions. In natural environments, they decompose similarly to fossil-based plastics, breaking down into smaller particles and MPs [5]. Biodegradable MPs have hydrophobic surfaces, enabling high adsorption of hydrophobic organic pollutants like pesticides, affecting their distribution and fate in agricultural areas [4].

This study investigated the adsorption of the broad-spectrum fungicide azoxystrobin (AZO) on pristine and aged MPs of PE, thermoplastic starch (TPS), and a copolymer of PBAT and PLA with additives, as well as the desorption of AZO from these MPs. Mulch sheets of each polymer were artificially aged in a climate chamber and naturally aged through one year of exposure to air and sunlight. Pristine and aged MPs were cut into particles smaller than 5 mm. Adsorption of AZO was tested in a $CaCl_2$ solution (0.0018 M) at a concentration of 5 mg/L and 1% MPs content. The adsorption study involved continuous stirring for 2 hours, with samples taken at intervals. MPs were then filtered, air-dried, and used for a desorption study in $CaCl_2$ solution (0.0018 M) and 10% ethanol, stirred for 8 days with samples taken periodically. AZO concentrations were determined using HPLC analysis (Agilent 1100 Series, DAD detector). Results showed higher AZO adsorption with TPS and PBAT/PLA (>85%), regardless of ageing, compared to PE. Aging did not increase the adsorption capacity of biodegradable mulch for AZO, unlike PE films. Desorption studies indicated that most AZO was desorbed from TPS and PBAT/PLA MPs compared to PE MPs. The study concluded that biodegradable mulch has a higher adsorption affinity for AZO than fossil-based PE mulch, and ageing does not enhance this affinity for biodegradable MPs as it does for PE films.

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P-EnvSaf-01

Reactivity of malodorous volatile organic sulfur compounds toward hydrogen sulfide

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Introduction

The presence of malodorous volatile organic molecules containing sulfur-sulfur bonds was documented in the water columns of natural aquatic systems [1,2] as well as in the drinking water distribution systems [3]. While processes leading to formation of these compounds were intensively studied during the last decades, kinetics and mechanisms of reactions which lead to their decomposition are poorly understood. In this work, the kinetics and products of the reactions of two linear molecules, dimethyl disulfide and dimethyl trisulfide as well as of cyclic polysulfide lenthionine (1,2,3,5,6-pentathiepane) with hydrogen sulfide at the environmental pH and temperature ranges were studied. It was shown that under environmental conditions ($\mathrm{pH} \geq 5$), the reaction of bisulfide anion (HS-) rather than that of hydrogen sulfide controls the overall reaction rates. The activation energy and the order of the reaction with respect to bisulfide anion is dimethyl disulfide < dimethyl trisulfide < lenthionine, while the order of the reaction with respect to organosulfur compounds is lenthionine < dimethyl trisulfide < dimethyl disulfide. The obtained results suggest that bisulfide anion is responsible for fast decomposition of organosulfur compounds in aphotic natural aquatic systems. The rates of the reactions between linear dimethyl polysulfides with bisulfide anion are higher than the rates of their reactions with cyanide and hydroxyl anions, but lower than the rates of their photodecomposition [4-7]. These results suggest that under aphotic conditions in sulfidic natural aquatic systems, the stability of dimethyl polysulfides is controlled by HS^- decomposition pathway. In addition, the cyclic polysulfides were shown to be more stable than their linear analogs. Products of the decomposition of dimethyl disulfide and dimethyl trisulfide include longer and shorter dimethyl polysulfides (but not dimethyl sulfide), methanethiol, elemental sulfur and inorganic polysulfides [8].

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P-EnvSaf-02

Human biomonitoring of hexavalent chromium: the potential role of epigenetics within chemical risk management in the workplace

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Introduction

Approximately 900,000 workers in the European Union are exposed to carcinogenic hexavalent chromium (Cr(VI)). Genotoxic effects, such as oxidative stress and DNA lesions, have been recognized as crucial events in the carcinogenic process of Cr(VI) compounds. Moreover, it has been suggested that, in addition to the induced genotoxic effects, epigenetic mechanisms like DNA methylation may contribute to the carcinogenicity of Cr(VI) compounds. Therefore, we investigated the epigenetic effects induced by occupational exposure to Cr(VI).

We applied a cross-sectional study design and used chromium in urine as the primary biomonitoring method for Cr(VI) exposure. Furthermore, the effect of occupational Cr(VI) exposure on 8-Hydroxydeoxyguanosine (8-OHdG), global DNA methylation and global DNA hydroxymethylation in blood was investigated. Workers with potential exposure to Cr(VI) were included (n=254). As controls (n=114), healthy adult (18–70 years) office workers from the same companies as the exposed workers (referred to “within-company controls”) or from other companies with no activities that were associated with Cr(VI) exposure (referred to “outwith-company controls”) were recruited.

Overall, each exposed subgroup displayed significantly higher mean urinary Cr levels than the total controls, the within-company controls, or the outwith-company controls ($p < 0.007$, Mann-Whitney test). The within-company controls had significantly higher internal exposure levels than the outwith-company controls ($p < 0.001$, Mann-Whitney test). The outwith-company controls exhibited significantly higher global DNA methylation levels and lower levels of 8-OHdG than all other exposure subgroups ($p < 0.01$, Mann-Whitney test).

Overall, these findings reinforce the results of exposure biomarkers, highlighting that in Cr-related industries, (office) workers' exposure to Cr is associated with detectable alterations in biological effect markers. Furthermore, characterizing epigenetic effects like global DNA methylation could improve risk management.

Acknowledgements

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P-EnvSaf-03

Potentially toxic elements and fatty acids in fish – health risk and benefit predictions for consumers

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Introduction

The assessment of benefits and risks for the consumers of pelagic fish is crucial for balancing the intake of healthy omega-3 and omega-6 fatty acids and potentially toxic elements (PTE). This study investigates the contents of PTE and fatty acids in 6 pelagic fish species. The investigated species from the Adriatic Sea are horse mackerel, sardine, round sardinella, anchovy, chub mackerel, and garfish. These fish species were investigated to assess health risks for consumers. The concentrations of 16 PTEs were measured by using inductively coupled plasma mass spectrometry (ICP-MS) and and content of 14 fatty acids was analyzed by gas-liquid chromatography (GLC). The measured PTE concentrations were used to assess health risks for consumers and risks of specific organs or organ systems. In addition, the benefit-risk of PTE and healthy fatty acids intake were investigated. The results indicated that a diet based on chub mackerel and round sardinella has the highest human intake of healthy fatty acids. Lower intake of PTEs in the gastrointestinal tract has a diet based on anchovy and round sardinella. The concentrations of PTE indicated low non-carcinogenic risk (HI 0.1–1). Anyhow maximum and outlier risk values (HIs) for horse mackerel and anchovy were higher than 1. Inorganic As was indicated as the primary contributor to total risks. Acceptable carcinogenic risks (CRs) were assessed for most of the investigated fish samples, but maximum CRs (that are some horse mackerel and anchovy samples) showed potential adverse carcinogenic effects for long-term and uncontrolled consumption in the diet. Observing the specific risks obtained in our study, there were low risks for cardiovascular, nervous and reproductive diseases, and for fish samples with maximum and outlier HI values, there was a risk (HI>1). However, there were no adverse effects on endocrine, hepatic and urinary non-carcinogenic disease development. There was an acceptable (1×10-4≥ R ≥ 1×10-6) risk for developing cancer of the nervous system and reproductive organs, while there was no risk for developing carcinogenic endocrine and hepatic illness. Benefit-risk assessments showed that inorganic As can cause the consumption of numerous pelagic fish samples from the Adriatic Sea may have a higher human health risk of PTE intake compared to the benefits of consumption of healthy fatty acids. This type of worst-case scenario health risk assessment study represents a precautionary measure for investigating the PTE pollution influence on aquatic ecosystems and human health, as well as the management in suggesting and dosing the pelagic fish in the human diet.

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P-EnvSaf-04

Tobacco sticks and nicotine pouches as an alternative to traditional smokeless tobacco products – comparison of their elemental composition

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Introduction

Nicotine is a chemical substance found mainly in tobacco leaves, widely used for centuries as a stimulant. The nicotine was isolated from the tobacco plant in 1828. However, it was only in 1893 that the chemical structure of nicotine was determined. The first complete synthesis of nicotine was carried out in 1904, which enabled the synthesis of nicotine in controlled laboratory conditions and opened the way to further research on this substance and its effect on the body. At the end of the 19th century, the first reports of the harmful influence of nicotine were published. In the following years, more studied were conducted regarding the risk of tobacco smoking. Finally, in 1964 smoking was linked to heart disease and lung cancer. There was also increasing attention to the problem of nicotine addiction. US Food and Drug Administration (FDA) in 1994 officially recognized it as an addictive substance. Today, although many harmful effects of nicotine are well-known, it is still legal and widely used in many countries around the world. We are also observing a dynamic development of tobacco substitutes for classic cigarettes on the market, which worsens the problem of tobacco addiction in a wider group of people. One of the alternative tobacco products is heated tobacco product. Tobacco sticks are very popular due to a different way of introducing nicotine without burning tobacco and with no unpleasant odor or ash. The system is equipped with a special heating device, i.e. a sharp ceramic plate, a metal tip made of stainless steel, which allows to place tobacco on the heating element. During use, the tobacco is heated to 350°C, generating steam that is transferred into the lungs. Heater cartridges differ in taste or type of tobacco mixture. Dried and ground tobacco leaves are shaped into special sheets. The sheets are fluted and turned into tobacco cork to release the best taste when heated [1-2]. Another products widely increasing its popularity are the pouches, whose roots date back to Sweden in the early 18th century. The Swedish version of pouches, which use is forbidden in Poland, is a moist, smokeless tobacco powder packed in a small sachet. Apart from ground tobacco, other components include salts used for preservation, bicarbonate sodium used to regulate pH, and numerous flavors to improve taste. Tobacco for the production of snus, unlike other tobacco products, is subjected to a pasteurization process, not fermentation. Most Scandinavian snus are produced in Sweden and are regulated by the Swedish Food Law. The nicotine content in this type of product varies depending on the manufacturer and is higher than in traditional cigarettes, typically containing from 8 to 14 mg of nicotine per gram of product. Stronger varieties can be found to contain up to 42 mg of nicotine per gram. However, typical nicotine pouches contain nicotine-based powders without tobacco and are recognized as new, tobacco-free products. In these products, nicotine salts are used, which are mixed with microcrystalline cellulose, various other components (including sodium carbonate and hydrogen carbonate), citric acid, and flavorings. Their attractiveness results from discreet use, variety of flavors, and higher nicotine content compared to traditional cigarettes. Nicotine is fast and efficiently delivered by placing the sachet under the top or lower lip, where it is absorbed. Even though tobacco-free pouches have been present on the Polish market since 2021, there are currently no proper legal regulations regarding their use, which raises concerns about increased addiction and health risks among young people, which is expected to change with a new year [3-4]. In this work, we have compared the results of the elemental analysis gathered for traditional smokeless tobacco products with the data acquired for new alternatives such as tobacco heated sticks and nicotine pouches against the limits considered as safe for so-called smokeless tobacco products. Before quantitative measurements, samples were treated with concentrated nitric acid and perhydrol and placed in a closed-pressure microwave energy system. The concentration of selected toxic elements was determined in the studied samples by the inductively coupled plasma optical emission spectroscopy ICP-OES.

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PY-EnvSaf-01

6PPD, 6PPD-quinone and other hazardous compounds in tire rubber particles from recreational surfaces

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Introduction

Crumb rubber, produced by shredding end-of-life tires, is a microplastic material used as infill in artificial turf sports fields and as flooring in playgrounds. In September 2023, the European Commission introduced a ban on the use of crumb rubber as infill, allowing manufacturers an 8-year transition period to comply with this regulation [1]. Tires contain various chemical agents such as antiozonants, vulcanizers, and crosslinking agents, which can also be present in these surfaces. These compounds are considered emerging contaminants due to their potential negative impact on the environment and human health. These chemicals can enter aquatic ecosystems directly through tire wear particles and indirectly through water leachates from crumb rubber surfaces [2]. Tire wear particles release 6PPD-quinone, a transformation product of the antiozonant 6PPD (N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine), into aquatic ecosystems, which has been associated with fish mortality [3]

This study proposes an analytical methodology to determine 11 emerging contaminants, including 6PPD and 6PPD-quinone, as well as vulcanizing and crosslinking agents, such as 1,3-diphenyl guanidine (DPG) or hexamethoxymethylmelamine (HMMM) [4]. The method is based on ultrasound-assisted extraction (UAE) followed by liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). Parameters affecting the extraction step were optimized: solvent, temperature and time. Once the method was validated for its analytical performance, it was employed to monitor these target compounds in a diverse range of crumb rubber samples from football pitches, playgrounds, and other urban surfaces. Additionally, alternative infill materials such as sand, thermoplastic elastomers, coconut fibres and cork granulate were collected and analysed. All target analytes were detected in the crumb rubber samples. High concentrations of 6PPD (up to 0.2 % w/w) were found in new synthetic turf. Moreover, 6PPD-quinone was present in all crumb rubber samples, reaching levels as high as 40 µg/g in football fields. The crosslinking agent HMMM was also detected in most crumb rubber surfaces, with concentrations up to 36 µg/g. In contrast, none of the target compounds were found in the alternative infill materials tested.

Acknowledgements

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PY-EnvSaf-02

Evaluation of dermal exposure to antiozonants and other tire rubber compounds present in recycled tire crumb rubber

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Introduction

One way to give a second life to end-of-life tires (ELT) is shredding them, obtaining recycled tire crumb rubber (RTCR) as a subproduct. This material is a microplastic widely used on daily surfaces and its main use is as infill in synthetic football fields. Its composition is not yet well characterized, but there are studies informing about the presence of polycyclic aromatic hydrocarbons [1] and tire related agents [2]. Among these tire related agents, N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine (6PPD) and its transformation product (2-((4- methylpentan-2-yl) amino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione), 6PPDq, are linked with the death of aquatic species [3]. In September 2023, the European Commission decided to ban the use of this material as infill in synthetic fields, but allowing a transitional period of 8 years [4].

As RTCR main use lies on surfaces to which children are highly exposed, this study tries to assess the content of chemical agents that reaches the children skin after exposure to RTCR. To achieve this purpose, two groups of children volunteers have been playing football on a synthetic football field. After that, they were asked to clean their hands employing sanitary wipes and cotton pads, subsequently extracted by means of two different extraction techniques, pressurized liquid extraction (PLE) and ultrasound assisted extraction (UAE). Simulated lab-samples were also prepared to assess the method analytical parameters. GC-MS/MS analyses were carried out showing that PLE and UAE both led to quantitative recoveries and good precision. The field samples revealed the presence of RTCR compounds on the skin of players, including 6PPD and 6PPDq, some of them in high amounts, demonstrating dermal contact as being a route of entry of chemical agents into the human body.

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PY-EnvSaf-03

Bioaccumulation and transformation of plastic additives in hydroponically grown plants: Implications for safe water reuse

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Introduction

Water scarcity is a critical global issue, exacerbated by climate change and increasing water demand. Reusing water, especially in agricultural irrigation, has become an essential strategy to address this scarcity [1]. However, reclaimed water often contains organic micropollutants, including plastic additives, that pose environmental and health risks [2]. These contaminants can persist through wastewater treatment processes and accumulate in crops, potentially entering the food chain [3]. Thus, it is essential to assess and mitigate these risks to ensure the safe use of reclaimed water in agriculture and protect public health.

This study explores the uptake and bioaccumulation of specific plastic additives and the formation of their transformation products (TPs) in a hydroponic system. The research focuses on Carex (Carex praegracilis) for phytoremediation and lettuce (Lactuca sativa) for crop production. The irrigation water was spiked with seven plastic additives commonly associated with textiles, packaging, and tire wear particles: benzotriazole-1H (BTR), bisphenol S (BPS), 1,3-dio-tolylguanidine (DTG), hexamethoxymethylmelamine (HMMM), benzothiazole (BTZ), tris(2-chloroethyl) phosphate (TCEP), and benzophenone-3 (BzP). Ultra-high-performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) was employed for targeted analysis of these additives in both water and plants to assess their uptake and bioaccumulation. Additionally, liquid chromatography-high-resolution mass spectrometry (LC-HRMS) was used for suspect screening to identify TPs.

The goal of this research is to improve our understanding of the behaviour of plastic additives in water reclamation scenarios, thereby contributing to effective phytoremediation techniques and safer agricultural practices.

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PY-EnvSaf-04

Fibrous microplastic influence on locomotory dynamics and entanglement in *Thamnocephalus platyurus* and *Brachionus calyciflorus*

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Introduction

Microplastic (MPs) pollution has become a growing environmental issue, with increasing quantities of these particles entering aquatic ecosystems [1]. While the ingestion of microplastics by aquatic organisms has been extensively studied, the morphological and behavioural impacts of MPs, particularly on invertebrates, remain underexplored [2]. Moreover, the entanglement of larger marine animals, such as fish and turtles, in macroplastic debris, is well-documented, while there is a significant gap in understanding how fibrous MPs interact with and affect zooplankton [3]. Very recently an entanglement of *Daphnia magna* by fibrous MPs through “Hook and Loop” action was proposed [4], however, it is unclear if such phenomena is relevant for other zooplankton species.

Present research investigates the interaction between two zooplankton species - *Thamnocephalus platyurus* (fairy shrimp) and *Brachionus calyciflorus* (rotifer), and fibrous polyester MPs with an average size of 322.37 µm ± 231.59 µm, at varying concentrations (0, 1, 10, 100 and 1000 items/mL). Zooplankton survival was evaluated after 24 hours of exposure, and alterations in locomotory dynamics, including swimming performance, movement patterns and entanglement frequency, were assessed. Behavioural changes were observed using light microscopy with digital imaging, and morphological assessments were further analysed through scanning electron microscopy (SEM).

The results revealed a tendency of fibrous MPs to adhere and entangle with the surface of *T. platyurus* in groups exposed to 100 and 1000 items/mL, with a frequency of 13% ± 5% and 17% ± 5%, respectively. Entanglement was observed on various body parts, including antennule, antennae, thoracopod buds, and telson, either as an individual fibres or clumps forming net-like structures. The swimming speed was significantly reduced in entangled individuals, while comparison of movement trajectories revealed visible differences between entangled and non-entangled *T. platyurus.* Additionally, SEM micrographs revealed physical damage to the thoracopod buds caused by entanglement. In contrast, no entanglement or adhesion was observed in *B. calyciflorus*, and there were no significant changes in swimming performance or movement trajectories among the exposed groups. No physical damage to the *B. calyciflorus* was detected. *T. platyurus* showed a significant decrease in survival at 1000 items/mL, while *B. calyciflorus* exhibited a progressive decrease in survival with increasing MPs concentrations.

The data indicate the significance of body size and morphology in the interaction between fibrous MPs and zooplankton. *T. platyurus*, being larger than the MPs and possessing numerous buds and spine-like structures, presents a greater surface area and therefore the higher number of structures are susceptible to entanglement. In contrast, *B. calyciflorus* is smaller than fibrous MPs and features a smooth, gelatinous surface that does not enable entanglement. This study advances our understanding of how fibrous MPs impact zooplankton behaviour and highlights the need for further research to explore the broader ecological implications of MPs contamination.

Acknowledgements

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PY-EnvSaf-05

Understanding the composition of the plastic-associated microbial community in Lake Geneva under different seasonal and spatial conditions and evaluating the biodegradation potential

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Introduction

In aquatic ecosystems, plastic degradation can result from aging processes such as weathering and/or biotic degradation by microorganisms (Jacquin et al., 2019). Bacteria, fungi, and algae can colonize and develop on the polymer surface forming biofilm. The study of biofilm community composition on plastic surfaces in freshwater ecosystems and their impact on the material after long incubation periods remains limited. In this project, our aim is to (i) characterize the bacterial and fungal communities on low-density polyethylene (LDPE) and polyethylene terephthalate (PET) in Lake Geneva and (ii) observe how plastic surface degradation evolves over time at different depths. LDPE and PET samples (2.5 x 7.5 cm) were incubated for ten months at two depths (2 and 30 meters) in Lake Geneva. Environmental parameters are measured continually through the platforms LéXPLORE. Biofilm DNA is extracted for Next-Generation Sequencing (16S rRNA for bacteria and ITS for fungi) and quantitative PCR targeting the alkane hydrolase gene genes (alkB). After biofilm removal, the plastic surfaces are analyzed using Fourier Transform Infrared (FTIR) spectroscopy to detect any chemical changes. In case of degradation, new oxidative functions appear, especially in carbonyls (Delacuvellerie, 2021). Additionally, contact angle measurements assess changes in surface hydrophobicity, expected to decrease with biofilm formation and the photooxidation (Rummel et al., 2021). Surface morphology is examined using Scanning Electron Microscopy (SEM). The results from NGS confirm that the biofilm community is strongly influenced by the lake depth gradient but not the type of plastic. At 2 meters depth, a dense biofilm including bacteria, fungi, and benthic algae develops on the plastic surface, with the biomass fluctuating significantly with seasonal changes. At 30 meters the biofilm grows constantly and is predominantly composed of bacteria and fungi. Contact angle measurements show a greater reduction of the hydrophobicity at 2 meters for both plastic types, which can be due to photooxidation or biotic factors. At 30 meters, PET's hydrophobicity remains stable, while LDPE's surfaces showed a significant decrease in hydrophobicity compared to virgin LDPE. Spectrum from FTIR analysis revealed a strong decrease in CH bonds (methyl group) and the appearance of new carbonyl peaks (1715 cm^{-1}–1649 cm^{-1}) on LDPE at 30 meters only, suggesting chemical changes on the surface. Noticeable porous cavities are observed with SEM imaging at 30 meters, confirming a possible plastic degradation after 10 months of incubation. To investigate the biodegradation potential of bacteria at 30 meters, we measure the abundance of the alkane hydrolase gene (alkB). A significant increase of alkB was observed on LDPE, whereas its abundance decreased on PET. The chemical properties of LDPE, an aliphatic hydrocarbon with lower crystallinity than PET, make it more susceptible to degradation by both abiotic and biotic processes.

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P-EnvTech-01

Sorption of pharmaceuticals using layered double hydroxides: considering environmentally relevant conditions

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Introduction

Widespread consumption of antibiotics, coupled with human activities, has resulted in their uncontrolled release into the environment. This pollution is of global concern, causing environmental toxicity and spread of antimicrobial resistance [1]. Antibiotics are emerging contaminants, not removed through traditional wastewater treatment approaches, hence advanced wastewater treatment technologies are required for their removal from environmental waters.

Layered double hydroxides (LDHs) are emerging as successful sorbents for wastewater treatment, attractive due to their low cost and simple synthesis. LDHs, also known as anionic clays, have tuneable physiochemical properties, which can be harnessed to design bespoke high-performing sorbent materials. Of particular interest, LDHs can be synthesised using a scalable continuous synthesis method, crucial to ensure movement up Technology Readiness Levels (TRL). Whilst a large body of literature is available for LDH performance for the removal of conventional pollutants (dyes, metals) from waters, their capability for removal of emerging contaminants, such as pharmaceuticals, at concentration representative of those present in the environment are limited [2]. Further, any commercial applications of LDHs as sorbent materials will require them to be successful in real environmental aqueous matrices, rather than in idealised 'clean' water. The complexity and variability of environmental waters is well known to impact removal of pollutants onto naturally occurring clays, but studies exploring whether this behaviour is analogous in LDHs are limited.

This work furthers the understanding of sorption behaviour of antibiotics in the presence of LDHs at environmentally relevant concentrations (µg/L) in wastewater effluent (WWE). Studies to date show removal behaviour is greatly dependent on pharmaceutical characteristics and composition of the water matrix. Our work shows a complex relationship between sorption of the antibiotic sulfamethoxazole and the characteristics of the water matrix [3]. Further, equilibrium removal of amoxicillin decreased from 94.5±0.1% in ultrapure water to 0 % in WWE. This inhibitory effect is due to multiple competing ions present in effluent, which preferentially sorb to the LDH. This work reinforces the importance of carrying out research in environmental waters early in the development of sorbent materials.

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P-EnvTech-02

Development of hybrid matrices with photothermal and catalytic functionalities for environmental applications

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Introduction

Water quality is crucial for human health and the stability of ecosystems. Phenolic compounds, which include dyes, pharmaceuticals, and plastic-derived substances, are among the most common pollutants. These compounds are typically resistant to biodegradation, making them highly persistent in the environment. Laccase, an enzyme with a broad oxidative spectrum against phenolic and aromatic compounds, presents a promising solution for wastewater bioremediation. However, its industrial application is limited by enzyme reuse challenges and heating requirements to achieve efficient catalysis. Immobilizing laccase within polymeric matrices offers a potential strategy to address these limitations. Additionally, incorporating plasmonic nanostructures may enable photothermal control of enzyme activity through a synergistic effect with 3D immobilization.

This study focuses on developing hybrid materials that combine photothermal and catalytic functionalities. Two materials were evaluated: organic polymeric hydrogels based on acrylamide and inorganic silica matrices produced via the sol-gel method. Gold nanoparticles (AuNPs) were incorporated into these materials to provide photothermal properties. AuNPs were synthesized using the Turkevich method and characterized in both uncoated and polymer-coated forms (PVP – polyvinylpyrrolidone, and PDADMACl – poly(diallyldimethylammonium chloride)). The PVP-coated AuNPs were successfully embedded into silica matrices during the condensation process, while in-situ synthesis of AuNPs was employed for the organic hydrogels. The photothermal properties of the immobilized AuNPs, including plasmonic wavelength and temperature increase under laser irradiation, were assessed. Laccase was used as a model enzyme for its catalytic capabilities and characterized in solution by examining its conformational state, thermal stability, and catalytic activity.

The results revealed that laccase incorporation into hydrogels altered the swelling properties of the material, and that in silica matrices, the enzyme maintained its structure, although a slight reduction in thermal stability was observed through fluorescence analysis. Both materials showed decreased enzyme activity after immobilization compared to free enzyme, as indicated by colorimetric assays. Despite the need for further optimization of enzyme stability and activity within the 3D matrices, this study establishes a foundation for the development of multifunctional hybrid materials, successfully co-immobilizing both nanostructures and enzymes in silica matrices.

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P-EnvTech-03

Adsorption of aqueous Hg(II) using activated carbons developed from agroforestry biomass: equilibrium and kinetics studies

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Introduction

Mercury is one of the most toxic heavy metals, since it can produce negative health effects at very low concentrations, and it is highly bioaccumulated and biomagnificated [1]. Mercury compounds could be present in polluted waters through natural and industrial processes. Thus, in the last decades continuous research efforts have been done to avoid mercury discharges and treat the mercury containing waters. This work was focused on the study of the removal of aqueous mercury by adsorption on activated carbon prepared from different sources of lignocellulosic biomass, by analysing the kinetic and equilibrium points of view.

Activated carbons are known as effective materials for mercury adsorption. The adsorbents can be produced from carbonaceous materials derived from petroleum, coal, tar, or polymers and, more recently, there is an increasing interest of valorising biomass waste by carbonization into activated carbons with suitable properties as adsorbents. Three types of lignocellulosic biomass produced in Spain, were selected to be used as raw materials: rice husk (RH), eucalyptus leaves (EL), and spent coffee grounds (SC). All the biomass samples were widely characterised following the European Standards to obtain proximate and ultimate analyses. The sieved powders (180-250 mm) were thermally pyrolyzed under a nitrogen atmosphere to obtain the corresponding char samples, which were chemically activated using different activating agents ($ZnCl_2$, KOH, and H_3PO_4). The influence of the pyrolysis temperature that was varied from 500 to 800 ºC on the properties of the activated carbons was evaluated and related to the aqueous mercury adsorption behaviour. To test the mercury adsorption behaviour, two types of batch experiments were carried out by modifying the contact time and the mercury initial concentration to obtain the kinetic profiles and the equilibrium adsorption isotherms at room temperature. Several theoretical models were used to fit the experimental results: pseudo first-order and pseudo-second order for kinetics, and Langmuir, Freundlich and Sips for equilibrium analyses.

The mercury adsorption capacity of activated carbons prepared from the studied biomass residues was very significant. It was found that the treatment of char with KOH solution produced the activated carbons with the highest Hg(II) adsorption capacities, which varied depending on the type of biomass in the order EL< SC < RH. Besides, these KOH-activated carbons exhibited a higher adsorption rate in comparison with those obtained from zinc chloride or phosphoric acid activation as previously reported [2]. The differences found in mercury adsorption behaviour can be explained considering the porous properties of activated carbons, which are microporous with a wide range of textural properties. As an example, BET surface area was influenced by the chemical activating agent, the pyrolysis temperature of the activation process, and the type of biomass. The increase of BET surface area of activated carbons yields both, a higher Hg(II) adsorption capacity and a higher adsorption rate. The values of mercury loading could be also related to the elemental analysis of activated carbons which is influenced by the chemical composition of the biomass source. For example, AC obtained from rice husk contains the largest amount of inorganic residue due to the ash content of rice husk biomass (related to alkaline, alkaline-earth metal oxides, and silica inherent to lignocellulosic biomass) compared to those obtained for spent coffee waste and eucalyptus leaves, respectively.

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P-EnvTech-04

Adsorption of carbamate pesticide desmedipham from aqueous solution using reactivated active carbon spheres

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Introduction

Human activities such as agricultural usage of herbicides, desiccants, and pesticides involving crop farming and industrial processes such as petroleum refining and combustion of fossil fuels, are contributing to the growing pollution of ground and surface water in amounts higher than the ecosystem can receive [1]. It has been proven that exposure of the organism to pesticides and their decomposition products can have carcinogenic and mutagenic effects, and the toxicity of pesticides certainly causes cell damage and the creation of metabolites harmful to the organism [2].

Desmedipham belongs to the broad-spectrum carbamate pesticides with neurotoxic influence, used to manipulate or control undesirable vegetation. However, extensive pesticide use in agricultural practices can lead to environmental pollution and human health issues [3]. Many studies have proven that lethal and sub-lethal effects have been described following desmedipham exposure in aquatic and soil organisms, even in more complex organisms such as rodents, amphipods, and fish. The high toxicity of the carbamate pesticide desmedipham places it in the group of easily accessible chemical compounds that can be used in crises such as terrorist acts or war for water pollution, which is an essential resource for survival in addition to food [4]. Adsorption was widely investigated as a process for dissolved or dispersed pollutants in untreated effluent. The effectiveness of the adsorbent depends on the porosity, surface area, number of available sites, and possible interactions with the target contaminant. The various possible adsorbents were used for wastewater treatment [4].

This study investigated the adsorption of desmedipham using the carbon (RAC) microspheres obtained from Saratoga™ filtering protective suiteactivated at 650℃ and with the density of used activated carbon between 180 and 220 g m^{-2}. These suits provide a minimum of one-day protection and more than 40 days of wear under battlefield conditions, including several washings cycles [5]. The dependence of pesticide removal efficiency of different initial parameters such as pesticide and adsorbent particles concentration, pH, and the temperature was studied. The kinetic study includes the pseudo-first, pseudo-second (PSO), and second-order kinetic models. Desmedipham removal using reactivated carbon was followed by ultraviolet-visible (UV-Vis) spectroscopy. The kinetics parameters of pesticide adsorption were monitored from 20 to 180 minutes. After 3 hours of the pesticide removal, equilibrium was established. According to the obtained results the kinetics for all adsorbents are best described using a second order kinetics model. At optimal conditions (C_{RAC}= 1 g/L, C_{DES}=2.33×10^{-5}, and pH 5), the adsorption capacity was qe = 29.649 mol g^{-1} × 10^{-8} and the adsorption rate was k = 4.3×10^{-4}g $mmol^{-1}$ min^{-1}, and activation energy was E_a=14.935KJ mol^{-1}.

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P-EnvTech-05

MgAl-layered double hydroxide particles for adsorptive removal of Acid Green 25 from aqueous solutions

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Introduction

Water pollution caused by organic dyes from textile industrial is a global environmental concern. Organic dyes are used for coloring textile, cosmetics, paper, and other, are non-biodegradable, carcinogenic and have trend accumulate in the human organisms and environment [1,2]. In recent years, the adsorption process as cheaper and efficient technology is widely used for water purification [1]. The development of adsorbents with high binding capacity, and affordable, and environmentally acceptable the same time is on the rise. Consequently, the new Layered Double Hydroxides (LDHs) materials due to simple and easy synthesis between two cationic metals, high surface area, porosity and active site can be used for removal anion dyes from water [2].

This work aims to study the textile dye adsorption efficiency on layered double hydroxide MgAl-LDH. A molar ratio of Mg to Al of 3:1 and a coprecipitation method were used for the synthesis of Mg-AL-LDH. The structural and chemical characteristics of MgAl-LDH particles were examined using the following techniques: pH at the point of zero charge (pHpzc), XRD, FTIR, FE-SEM with EDS analysis and XPS. The MgAl-LDH adsorbent demonstrated adsorption capabilities of 170.9, 176.1, and 181.2 mg $g^{-1}$was obtained from Langmuir model fitting at 25, 35, and 45 °C, respectively, for the Acid Green 25 (AG-25)dye removal.The adsorption of AG-25 was spontaneous and endothermic, as evidenced by thermodynamic characteristics. The results showed that, in the case of AG-25, both physisorption and chemisorption was the operative processes. Intra-particle diffusion was identified as the rate-limiting phase as obtained from kinetic study. A circular economy has been successfully implemented with little environmental effect thanks to the development of wastewater treatment technologies that have the potential to be commercially viable.

Acknowledgments

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P-EnvTech-06

Photocatalytic activation of hypochlorite with graphitic carbon nitride under by simulated sunlight irradiation

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Introduction

The increasing concern over water scarcity is challenging research to find new solutions for water treatment. The presence of organic contaminants in surface waters results from the inefficiency of conventional water treatment technologies. Heterogeneous photocatalysis has been shown as a promising solution as a simple method for the oxidation of chemical compounds [1]. In particular, graphitic carbon nitride (g-C_3N_4) can be activated by visible-light or simulated sunlight irradiation and lead to the degradation of a variety of organic pollutants.

In this work, we aimed to synthesise and optimise a g-C_3N_4 material [2] and assess its direct photochemical activation of hypochlorite for the removal of acetaminophen (ACTP). The impact of catalyst-to-oxidant ratio was investigated, as well as the influence of the matrix components (mineral salts and organic matter). Scavenging experiments were also performed by adding trapping agents into the solutions.

The effect of distinct mineral salts and pH level was investigated, revealing the integrated system was not as significantly hindered as the individual processes. The presence of organic matter (10 ppm of humic acid) was the most impactful interferent, reducing ACTP removal down to 76% in 1 h.

The combination of a metal-free photocatalyst, simulated sunlight and hypochlorite - Figure 1 - improved the removal of acetaminophen in synthetic mineral water.

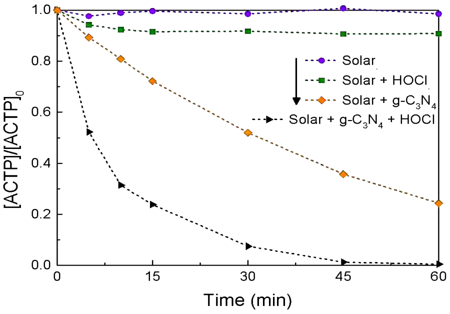

Figure 1. Removal of acetaminophen (ACTP) from mineral water by simulated sunlight, photocatalysis, chlorination and integrated process.

Acknowledgements

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P-EnvTech-07

TEVA@pipette-tip for on-site SPME of uranium employing a portable smartphone-based colorimetric platform for detection

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Introduction

Uranium is a toxic and radioactive element present in the environment, particularly in water sources due to mining, industrial activities, and natural processes [1]. Its accumulation in ecosystems and drinking water poses a significant risk to human health and the environment. Therefore, continuous detection and monitoring of uranium in water are essential to assess its impact and mitigate risks [2].

This work presents a miniaturized and low-cost methodology (Fig.1) that combines uranium SPME using a 3D-printed pipette-tip, which contains a matrix of cubes inside coated with TEVA resin [3]. After the extraction/preconcentration step, a colorimetric reaction with Arsenazo-III [4] is carried out, using a 3D printed platform equipped with wells for samples/standard/blanks and a homogeneous LED-based lighting system. Detection is performed using a smartphone to capture images of the sample, which are then analysed through RGB image decomposition [5], allowing the accurate quantification of uranium in aqueous samples.

The developed portable platform is presented as an alternative methodology for the on-site analysis of water samples, capable of reaching the detection levels established by regulations, while significantly reducing the high costs associated with conventional methods and streamlining the management of water resources.

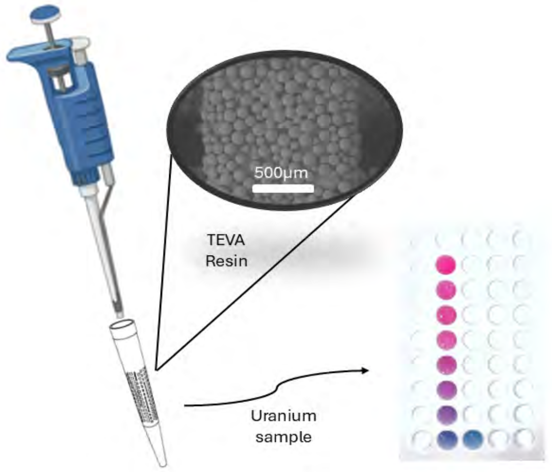

Figure 1. Scheme of SPME of uranium by TEVA@pipette-tip and its colorimetric detection.

Acknowledgements

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P-EnvTech-08

Phytoremediation of PFAS compounds using wheat seeds treated with alternating electric fields

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Introduction

Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals that enter the environment through human activities and are commonly found in products such as non-stick cookware and firefighting foams. Due to their chemical and thermal stability, PFAS persist in the environment and bioaccumulate in humans and animals, posing significant health risks [1]. Also, their remediation from contaminated soil and water is a very challenging task. Phytoremediation, an eco-friendly and cost-effective method, leverages the natural ability of plants to absorb and stabilize contaminants. This approach can address PFAS contamination by utilizing plant root systems to remove low concentrations of pollutants, making it an attractive alternative to traditional physical and chemical methods [2]. Phytoremediation not only helps to restore ecosystems but also prevents secondary pollution and minimizes landscape damage by stabilizing soil and supporting microbial activity. Combined with adsorption techniques, phytoremediation offers a promising solution to address the growing environmental concerns surrounding PFAS contamination [3].

It is interesting to mention that over the years more attention has been devoted in developing physical treatments of seeds in order to either substitute or at least improve conventional methods. Among those, usage of magnetic fields for seed pre-sowing treatments is most commonly found in the literature. Since application of alternating electric field (AEF) could offer easier scalability to larger volumes, in our previously performed preliminary experimental study [4] the influence of AEF (in the frequency range up to 1 MHz) was studied on wheat seed growth and germination. Mentioned study showed not only that AEF may enhance both seed germination and plant growth, but also it caused statistically significant differences (within 95% significance level) between control and treated seeds in chlorophyll a, b and total chlorophyll content in wheat lives, as well as in Normalized Difference Vegetation Index and Greenness Index [4].

In the present study, we combined phytoremediation with AEF in order to evaluate influence of AEF on PFOA (perfluorooctanoic acid) uptake by wheat. PFOA was used as a representative of PFAS compounds. After 48 hours of AEF treatment [4], wheat (*Triticum aestivum*) seeds were planted in hydroponics and exposed to high PFOA concentrations (1 ppm). PFOA accumulation was monitored using targeted LC/MS/MS analysis. A control group of untreated wheat seed was grown in parallel for comparison.

This study confirmed previous results [4] that wheat (*T. aestivum*) treated with alternating electric fields exhibited faster seed germination compared to untreated seeds. After the harvest, targeted LC/MS/MS analysis of PFOA revealed a significant reduction of PFOA in the hydroponic solution (over 80%), indicating effective uptake by the plants. Further analysis showed notable PFOA accumulation within the plant tissues, with the majority of the compound being localized in the roots (75%). In comparison, the stems contained lower levels of PFOA, suggesting that the roots play a primary role in absorbing and retaining the contaminant. While the use of alternating electric field increased the speed of seed germination, there was no difference in PFOA accumulation in treated seed compared with the untreated. AEF did not impact the distribution of PFOA within the plant, with approximately 75% of accumulated PFOA remaining in the root. These findings suggest the potential use of wheat for phytoremediation of environment contaminated with PFOA, however the application of AEF for increasing the PFOA accumulation needs to be optimized further.

Acknowledgements

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P-EnvTech-09

Boosting reef restoration: optimization of coral growth with electrochemical technologies

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Introduction

Coral reefs have been suffering intense degradation during the last decades. The worsening of their conditions due to environmental aggressions has triggered the debate on the need for restoration measures. Several methodologies for coral reef restoration have been proposed. The most common methods are: direct coral transplantation, coral nurseries or artificial reef fabrication.

An advanced method to achieve this is the electrochemical deposit of minerals on metallic supports, obtained by electrolysis of seawater. When a reduction potential is applied to an electrically conductive structure, electrochemical reactions occur, which cause an increase in pH in the vicinity of the electrode. This promotes the deposition of dissolved species in the seawater, mainly calcium carbonates and magnesium hydroxides.

According to several authors, corals transplanted on these electrodes experience increased growth rate, but the results are controversial. A reason for the inconsistent result is the great deficit on fundamental research on the processes that occur when seawater electrolysis is performed. Almost all the results in the literature show measurements in the open sea and hardly any results are found for electrolysis under controlled laboratory conditions or in aquaria.

Preliminary studies on the electrochemically stimulated growth of the coral species *Echinophyllia sp*. a coral of the order *Scleratinia* and family *Lobophylliidae* are presented. It is found in the Indo-Pacific, near Arabian Seas, the Indian Ocean and the western and central Pacific Ocean. It is a genus of encrusting, lamellar or foliaceous corals with a foliaceous, round or oval shape. This type of coral has been selected because it is one of the top ten species used in coral reef restoration projects and is classified as slightly threatened by the International Union for Conservation of Nature (IUCN) Red List of endangered species. The study assumes that a coral with a greater horizontal growth will have the growing edges in contact with the zone of maximum $CaCO_3$ concentration, thus stimulating its growth. The study was carried out in the marine aquarium of the Group of Electrocatalysis and Polymer Electrochemistry (AqUA-GEPE, Fig. 1).

Fig. 1: Reef Research Aquarium of the Group of Electrocatalysis and Polymer Electrochemistry (AqUA)

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P-EnvTech-10

Evaluation of the solar photocatalytic performance of graphitic carbon nitride (g-C_3N_4) on the removal of the insecticide acetamiprid in water

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Introduction

Graphitic carbon nitride (g-C_3N_4) is a metal-free semiconductor largely used in photocatalysis due to its stability, low-cost synthesis, and photoactivity in the visible light range (band gap ~2.7 eV). As a graphitic material, the exfoliation process enhances its photocatalytic performance by improving the textural and optical properties, and charge transport efficiency [1]. The precursor used in the synthesis is critical in determining the material's final properties and suitability for subsequent exfoliation. In this research, g-C_3N_4 derived from urea and melamine were thermally exfoliated and their performance in the solar photocatalytic degradation of 20 mg L^{-1} acetamiprid (ACP) in water solution was studied. ACP is an effective neonicotinoid insecticide widely used to control common insect pests. However, its presence in water bodies can be very harmful to aquatic species. On this basis, the present work aimed to investigate the effectiveness of heterogeneous photocatalysis with g-C_3N_4 to achieve ACP degradation in water and determine the transformation products (TPs) formed from the parent compound throughout the oxidation reaction [2].

The reactions were performed under simulated solar radiation. For evaluating the degradation kinetics of ACP and compare the materials performances, we developed a HPLC-HRMS method using a reverse phase column for chromatographic separation coupled through an ESI source to a high resolving power mass spectrometer (Ultimate Dionex 3000 - Orbitrap Fusion Tribrid, Thermo Scientific, Bremen, Germany). With this HPLC-HRMS method we identified and characterised TPs arising from ACP. The chromatographic separation of TPs was achieved using 0.1% formic acid (eluent A) and acetonitrile (eluent B) from 5 to 100% of B in 25 min. The orbitrap mass analyzer was used for the acquisition of full mass and MS/MS spectra with a resolving power of 60 and 50 k, respectively. The characterization of the ACP fragmentation pathway was the initial step to propose the structural formulas of the TPs applying the rules for the identification level [3].

The exfoliation temperature of g-C_3N_4 materials highly influenced their photocatalytic performance for ACP removal. The optimal conditions were 450 ºC and 500ºC, for urea and melamine precursors, respectively (U450 and M500 samples). Similar kinetic profiles of ACP degradation were observed with both catalysts, although U450 showed a higher reaction rate than M500 achieving 50% and 20% of ACP depletion, respectively, after 180 min. Regarding the TPs, the good resolution of chromatographic separation and the high resolving power of the orbitrap allowed identifying 23 TPs, some of them with more than one isomer. Moreover, the same identified TPs were detected with both materials, although their concentration values were significantly higher in the case of using U450 compared to those obtained with M500.

Acknowledgements

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P-EnvTech-11

Biosoprtion of amoxicillin and diclofenac from wastewater on modified biochar from buckwheat hulls

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Introduction

Persistent pharmaceutical pollutants (PPPs) at concentrations ranging from nanograms to micrograms per liter have been identified as potential endocrine disruptors that mimic growth hormones posing a significant risk to public health when present in drinking water. In this study, biochar derived from buckwheat hulls and functionalized with H_3PO_4 was evaluated for its efficacy in removing amoxicillin (AMX) and diclofenac (DCF) from model solutions and synthetic wastewater. Batch experiments were performed to evaluate the effects of variables such as biosorbent concentration (2 - 12 g dm^{-3} and 0.2 - 6 g dm^{-3}), contact time (5 - 360 minutes), initial AMX and DCF concentrations (5 - 50 mg dm^{-3}) and pH (2 - 10). The results showed that increasing the biosorbent concentration resulted in higher AMX and DCF biosorption per unit mass and improved overall removal efficiency. For AMX, higher initial concentrations (10 - 40 mg dm^{-3}) resulted in higher biosorption per unit mass, likely due to a stronger driving force of the adsorbate on the biosorbent, although at 50 mg dm^{-3} the biosorption efficiency decreased. In the case of DCF, increasing the initial concentration had no significant effect on the removal efficiency, which is probably due to the saturation of the active sites on the biochar. The biosorption of AMX was more effective in synthetic wastewater than in model solutions, while the biosorption of DCF was not effective in synthetic wastewater. The biosorption process was well described by both the Freundlich and Langmuir isotherm models as well as by the pseudo-second and pseudo-first order kinetic models.

P-EnvTech-12

The influence of pressure changes on the contents and composition of torrefaction liquid products from microalgal biomass

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Introduction

Algae are potential feedstock for the production of bioenergy and valuable chemicals. After extracting specific value-added products, algal residues can be further converted into biogas, biofuel, and biochar through various thermochemical treatments such as conventional pyrolysis, microwave pyrolysis, hydrothermal conversion, and torrefaction [1]. Torrefaction is a thermochemical process of conversion, also known as mild pyrolysis. It typically occurs under oxygen-free and atmospheric pressure conditions at temperatures between 200 °C and 300 °C and a time of 10–60 min [2].

This preliminary study investigates the composition and quantity of liquid products obtained from microalgal biomass through mild pyrolysis, i.e., torrefaction. The microalgal biomass used for this experiment consists of several types of microalgae, among which *Scenedesmus sp.* predominates, cultivated in pools for microalgal growth stimulation. Pyrolyses were performed in an autoclave at a temperature of 250 °C and different pressures under nitrogen for 4 h. The initial mass of microalgal biomass was 1 g. Liquid pyrolysis products were extracted with hot chloroform, while gaseous products were not analyzed. Liquid pyrolysates were separated into saturated and aromatic hydrocarbons using column chromatography (adsorbents: SiO_2 and Al_2O_3). The saturated hydrocarbons were eluted with *n*-hexane and aromatics with a mixture of *n*-hexane/CH_2Cl_2. The gas chromatography-mass spectroscopy (GC-MS) analysis was performed to separate and identify hydrocarbons.

Yields of liquid pyrolysates and hydrocarbons obtained by torrefaction of microalgae are given in Table 1.

Table 1. Temperature, pressure, and yields of liquid pyrolysates and hydrocarbons during torrefaction

Samples	T (°C)	P_0 (bar)	P_1 (bar)	Yields of liquid pyrolysates [mg]	SHC (%)	AHC (%)
1	250	/	/	28.1	4.59	7.14
2	250	5	9	143.1	4.00	7.00
3	250	14	25	520.9	5.34	5.83

Note: *P_0—initial pressure; P_1—working pressure; /—without pressure; SHC—saturated hydrocarbons; AHC—aromatic hydrocarbons.*

The results obtained in the three pyrolysis experiments show that pyrolysis yields are directly proportional to pressure (Table 1). On the other hand, a very similar percentage composition of saturated and aromatic hydrocarbons was observed (Table 1).

The GC-MS analysis of liquid pyrolysates at different pyrolysis pressures indicated the presence of a complex mixture of organic compounds. The *n*-alkane distribution in soluble organic matter extracted from the microalgae is characterized by pronounced *n*-C_{17} domination (~40 % within the total *n*-alkane distribution). Pyrolysates 1 and 2 have similar *n*-alkane distributions in which *n*-alkanes C_{23}–C_{27} are predominant. In pyrolysate 3, in addition to the mentioned mid-chain *n*-alkanes, a dominant member of the *n*-alkane distribution is *n*-C_{29}. Generally, most probably precursors of these compounds are lipids from microalgal biomass.

This research showed that the change in pressure during torrefaction significantly affects the amount and composition of liquid pyrolysates. Further experiments are planned to optimize the process of conversion of microalgae into biofuels and potentially valuable chemicals.

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P-EnvTech-13

Fluorescent nanocomposite eutectogels: a new class of materials for potential environmental sensing applications

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Introduction

Polymer gels are a very interesting category of materials with an attractive combination of solid and liquid properties. Researchers have directed a great attention to these materials because of their adaptable nature and their wide range of potential uses in different fields. Recent advances in materials science have led to the development of new types of gels, such as ionogels and eutectogels, which utilize the unique characteristics of ionic liquids or deep eutectic solvents (DES) to enhance the functionality and versatility of traditional gel systems.

DESs are formed by specifically chosen combinations of hydrogen bond donors and acceptors, offering an eco-friendly and adaptable platform for material design and synthesis. Their distinct properties, such as low volatility, biodegradability, and compatibility with various chemical compounds, make them highly attractive for numerous applications. When DESs are integrated into polymer matrices, they give rise to eutectogels (EGs), which enhance the mechanical and structural properties of gels while also allowing the incorporation of functional additives for tailored functionalities. Thus, the incorporation of fluorescent nanoparticles would endow these materials with luminescent properties that could be used, in addition to other applications, for the development of optical sensors.

In this study, we focus on the synthesis and characterization of a novel class of materials that combine the fluorescent properties of conjugated polymers-based nanoparticles (CPNs) with the structural framework of EGs. Specifically, we incorporate the polyfluorene derivative poly[(9,9-di-n-octylfluorenyl-2,7-diyl)-alt-(1,4-benzo-{2,1,3}-thiadiazole)] (F8BT) in EGs prepared via a simple and rapid protocol through UV-induced in situ radical polymerization. The monomer 2-hydroxyethyl methacrylate (HEMA) was used as a precursor, dissolved in a ChCl:ethylene glycol DES along with the crosslinker ethyle glycol dimethacrylate (EGDMA), the photoinitiator and the CPNs to obtain the fluorescent nanocomposite EGs.

The synthesized materials were extensively characterized by evaluating their fluorescent properties, exploring how these properties respond to different compounds.The findings reveal that the eutectogels emit fluorescence at 550 nm, with the signal remaining stable for several weeks. This contrasts with the behavior observed when F8BT CPNs are incorporated into hydrogels, where aggregation occurs, rendering them unsuitable for practical applications [1]. In addition, the fluorescence intensity of EGs was found to be quenched by certain explosives, such as picric acid (TNP), which dissolves easily in water and poses a rapid contamination risk when released into the environment. The fact that the material selectively detects this compound against other known explosives such as TNT suggests its potential use as TNP sensor. Initial experiments were also conducted to test the feasibility of using the nanocomposite eutectogels to encapsulate enzymes like alkaline phosphatase. These tests showed that the enzyme retained its activity, which could be monitorized through changes in the eutectogel's fluorescence. This result suggests that, with further optimization, the material could also be applied for detecting aqueous pollutants that act as enzyme inhibitors, such as phosphate derivatives.

Acknowledgements

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P-EnvTech-14

Synthesis, characterization, and photocatalytic activity of spinel oxide materials

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Introduction

In recent decades mixed spinel oxides have received considerable attention for photocatalytic degradation due to their magnetic and optical properties [1]. This study investigates the development of $Co_{0.5}Zn_{0.5}Al_2O_4$ spinel oxides photocatalysts from layered double hydroxides Co-Zn-Al/CO_3 precursor by calcination at 300, 400, 500, 600, 800, and 1000°C. The catalysts were characterized using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscope (SEM) coupled with energy dispersive X-ray analysis (EDX), and thermogravimetric analysis (TGA) coupled with differential thermal analysis (DTA). The photocatalytic efficiency of the prepared materials was tested by photodegradation of methyl orange azo dye as a model of textile contaminants under UV irradiation. The effect of various operational factors such as irradiation time, initial pH, catalyst dose, methyl orange concentration and reuse were studied. The enhancement of the photodegradation was strongly dependent on the calcination temperature. A synergic effect between the adsorption and photodegradation was observed. After 50 min of irradiation, the catalyst calcined at 400°C showed the highest efficiency (98.2%). The recycling experiments of the optimal photocatalyst indicated its high stability after five cycles.

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PY-EnvTech-01

Preliminary study of waste *Paeonia tenuifolia* L. usage for lead ions removal from wastewater

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Introduction

The possibility of using waste stream and converting it into a useful material for the application in environmental engineering was the goal of this research. Cellulosic, natural, materials have attracted the attention of many researchers, due to their properties such as the plentiness of functional groups, readily biodegradation, wide abundances, etc [1]. They found application in biomedicine, biotechnology and biosphere remediation. Therefore, in this work, *Paeonia tenuiofolia* L. petals that have undergone hydrodistillation and extraction of bioactive components were applied as adsorbents for removing lead from wastewater. Since the ore processing, as a main source of lead pollution, is in the expansion worldwide, detected values of Pb^{2+} ions could be increased in effluents from smelters and mines. The material exhibited structural stability and consistency. Fourier-transform infrared spectroscopy (FTIR) showed changes in material after adsorption of Pb^{2+} ions on material surface, demonstrating its efficient removal from water solution. Scanning Electron Microscopy (SEM) gave better insights of material morphology. After 24 hours, the removal efficiency of the observed metal ion was 70%. Compared to the raw petals (before the hydrodistillation process), the obtained removal efficiency was 60%. These preliminary tests showed that this plant has a high adsorptive capacity and affinity for lead ions (calculated value for material after hydrodistillation was 67.5 and for material prior hydrodistillation was 57.5 mg/g). Given that the cultivation of medicinal plants is on the increase, both in Serbia and throughout Europe [2], this material has a future as a useful adsorbent. In this way, the usage cycle would be closed and it would significantly contribute to the circular economy and sustainable development, globally.

Acknowledgements

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PY-EnvTech-02

Remediation of water polluted by potentially toxic elements using biochar from corn and tomato

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Introduction

Biochar is a carbon-rich material with an interesting structure, a large surface and different pore sizes. Because of pores' presence, interesting surface area, and present functional groups, biochar is suitable to be used as an adsorbent in water polluted with potentially toxic elements. The aim of this research was to follow adsorption capacity of biochar from different type of biomass. In this research, we performed experiments with fresh and salt water, which are polluted with different elements. The biochars are obtained by pyrolysis of agricultural waste of corn and tomato. Obtained biochar was fully characterized before its usage as an adsorbent. BET analysis showed that the biochar from corn has surface area of 41.04 m^2/g, whereas tomato biochar has 198.21 m^2/g. Solutions of potentially toxic elements are made in three different concentrations: 20 mg/l, 15 mg/l, and 10 mg/l. Samples were stirred with biochar for 30 minutes and then filtered. These filtrates are collected and analyzed by ICP-OES, to determine the concentration of each element in them.

Concentrations of some elements like Al, Ba, Cr, Cu, Fe, In, and Tl are drastically reduced, even for so short time of mixing biochar as an adsorbent with polluted water. On the other hand, elements like Ag, Bi, Ga, and Zn are totally removed from polluted water in many trials. Also, it is important to notice that tomato biochar showed better adsorption characteristics, by removing higher concentrations of elements from polluted water, relative to corn biochar, which had a slightly lower adsorption capacity. This is expected because of the much higher surface area of tomato biochar relative to the low surface area of corn biochar.

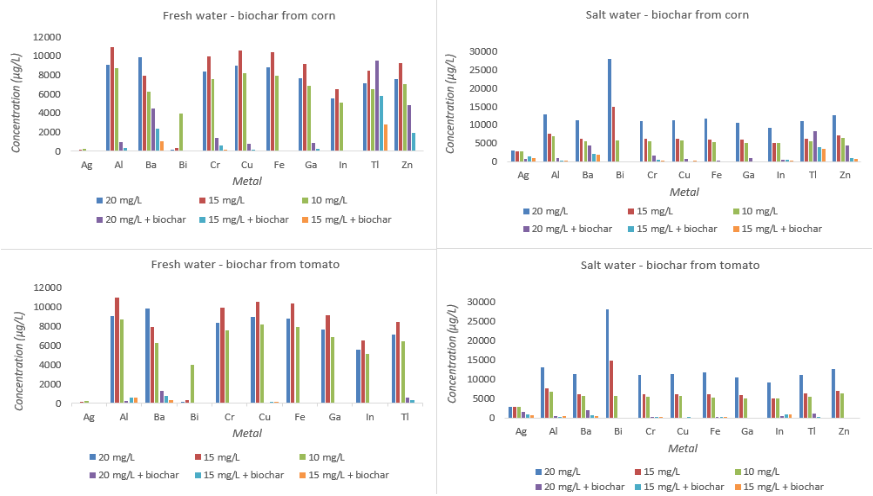

Fig. 1. Concentrations of potentially toxic elements before and after remediation of polluted water using biochar stirring for 30 minutes.

Acknowledgements

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PY-EnvTech-03

A new approach for temporal monitoring of reactive oxygen species in advanced oxidation processes

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Introduction

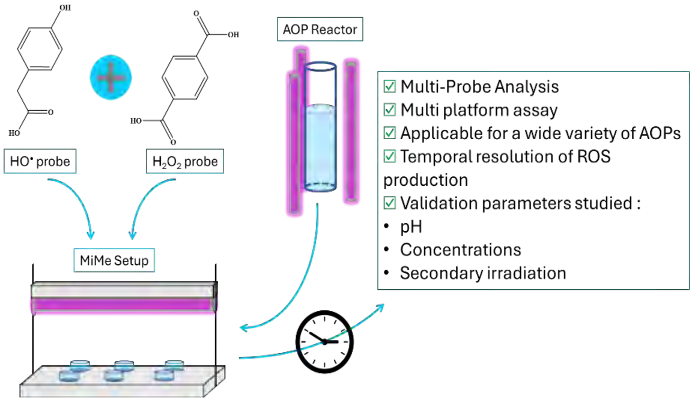
Advanced Oxidation Processes (AOPs) are an effective method for water remediation, particularly in reducing concentrations of refractory pollutants [1]. Most AOPs rely on the production of reactive oxygen species (ROS) to degrade organic contaminants through oxidative reactions, ultimately leading to complete mineralization. However, despite their widespread use, the mechanisms of many AOPs remain poorly understood due to the highly reactive and short-lived nature of ROS.

In this study, we introduce a novel approach for real-time tracking and quantification of ROS concentrations during AOPs, providing temporal resolution through the use of specific fluorescent probes that react with distinct ROS [2,3]. This time-resolved data enables a deeper understanding of ROS evolution and pollutant degradation pathways, shedding light on the mechanistic aspects of AOPs.

Our method, the Mirror-Method (MiMe), employs a multi-probe strategy to replicate the AOP process in parallel mini-photoreactors. Aliquots from the primary AOP reactor are mixed with specific probes and irradiated separately to generate ROS alongside their corresponding probes. This approach enables simultaneous monitoring of multiple ROS without disrupting the main reactor, addressing the limitations of in-situ methods, such as significant probe degradation, the inability to use multiple probes concurrently, and the absence of temporal evolution data.

The MiMe method has been optimized to track key ROS, including hydroxyl radicals and hydrogen peroxide, providing detailed insights into their temporal evolution during AOPs. Additionally, it captures secondary ROS generation and precursor formation, which are often difficult to observe using traditional techniques.

Extensive validation of the MiMe method has been conducted, assessing factors such as probe concentration, secondary irradiation time, pH effects, and the type of AOP. The method is adaptable to various analytical platforms, including fluorescence spectroscopy for rapid measurements and high-performance liquid chromatography (HPLC) for enhanced signal resolution when multiple probes are used simultaneously.



Acknowledgements

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PY-EnvTech-04

Removal of venlafaxine and diclofenac from drinking water using a *Spirulina*-based carbon bio-sorbent and a commercial adsorbent

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Introduction

Following the implementation of the revised European Drinking Water Directive (EU 2020/2184 [1]), more stringent standards for drinking water quality were set since ensuring access to safe drinking water is a critical public health priority. In particular, there is an urgent need to remove contaminants of emerging concern (CECs) from water supplies. The present study evaluates the effectiveness of a promising biosorbent based on *Spirulina* and compares it to a commercial tap water filter. A *Spirulina* material was prepared following the protocol established by Pedrosa *et al.* [2] and characterised by different techniques. Batch adsorption assays were performed in order to evaluate the removal of two CECs, diclofenac and venlafaxine, spiked in drinking water. Samples were analysed by high-performance liquid chromatography (HPLC) with fluorescence detection. Adsorption capacities were determined by adjusting known adsorption isotherm models to the obtained data. The *Spirulina*-based biosorbent, which was previously proved to be biocompatible [3], showed a high surface area and allowed for faster and higher removals than the commercial material.

Acknowledgements

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PY-EnvTech-05

Functionalized porous sponge of chitosan/alginate with hydrophobic eutectic solvent for paraben extraction in water

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Introduction

Parabens have been widely used in many personal care products due to their chemical stability, affordability, broad-spectrum antimicrobial properties, and low potential for triggering allergic reactions. Nevertheless, their use has steadily increased, leading to higher concentrations of parabens in the environment [1]. . Water serves as a significant reservoir for these chemicals, which are frequently detected in wastewater and surface water sources at elevated concentrations, reaching up to 100 μg L^{-1} [2]. This raises significant concerns about the impact of parabens on human and animal health. Parabens have been classified as endocrine-disrupting contaminants, and exposure to them has been linked to childhood obesity, breast cancer, and dysfunctions of the central nervous and immune systems [3].

Due to the importance of accurate quantification, various methods have been developed to measure parabens, including solid-phase extraction and liquid-phase extraction, among others. These techniques commonly use environmentally unfriendly extraction solvents, such as methanol, chloroform, and carbon tetrachloride. To address these challenges, deep eutectic solvents (DESs) have emerged. DESs are formed by combining hydrogen bond acceptors (HBAs) and hydrogen bond donors (HBDs) to produce a homogeneous liquid. Nowadays, hydrophobic DESs are gaining attention because they form a separate organic phase that can be easily isolated from the aqueous phase, making them useful in various extraction techniques [4].

Based on the above, a porous chitosan/alginate sponge was developed and functionalized with a hydrophobic eutectic solvent for the determination of parabens in aqueous matrices, followed by subsequent analysis using ultra-high-performance liquid chromatography with a diode array detector (UHPLC-DAD). The proposed methodology involves the use of menthol, thymol, and camphor as hydrophobic DESs, offering the advantages of being inexpensive, non-hazardous, and biocompatible. These DESs are used for the functionalization of chitosan and alginate as biodegradable adsorbent material, resulting in a device with increased surface area and enhanced adsorption performance.

Figure SEQ Figure * ARABIC 1 Scheme of parabens extraction using the chitosan/alginate sponge functionalized with eutectic solvent.

Acknowledgements

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PY-EnvTech-06

Treatment of industrial wastewater with a high content of nitrogen compounds in the simultaneous nitrification and denitrification system

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Introduction

Nitrogen and phosphorus compounds contribute to eutrophication of natural waters, leading to excessive bio reproduction in recipients and poor water quality. This study focuses on developing an effective system for treatment of industrial wastewater generated from nitrous oxide (N_2O) production. Gaseous N_2O is widely utilized worldwide. The primary application lies in medicine, particularly in surgery and dentistry, owing to its anesthetic properties. Additionally, it is used as an oxidizing agent in a number of selective oxidation processes (fuel combustion, rocket engines), and plays essential role in the food industry for purposes such as food cooling, freezing, storage, as well as a food preservative, additive (E942), propellant, and packaging gas [1]. The industrial production of N_2O is based on the thermal decomposition of a hot solution of ammonium nitrate. A significant amount of water is used in this process and also for treatment of the obtained gas. After the production process, a large amount of wastewater remains, containing high levels of nitrogen compounds such as ammonia, nitrates, nitrites, as well as total nitrogen and others. The wastewater needs to be treated to reduce the concentrations of these compounds below the maximum allowable concentration, ensuring it reaches a level suitable for discharge into the sewer system or natural recipient. This research involved simultaneous nitrification and denitrification (SNdN) within a single bioreactor, equipped with jet aeration. SNdN technology can offer significant advantages compared to conventional methods involving separate nitrification and denitrification reactors, resulting in reduction of operating costs and enhanced efficiency in wastewater treatment. It entailed experimental determination of the nitrogen transformation, monitoring process parameters, and assessing their impact on nitrification and denitrification efficiency to meet legislative emissions standards while maximizing process efficacy. The unequal distribution of dissolved oxygen (DO) inside the sludge floc creates an aerobic and anoxic zone and thus enables the simultaneous activity of nitrifying and denitrifying bacteria. The DO should be maintained in the range of 0.15 to 0.35 mg/l in the SNdN reactor in order to achieve a balance between these two processes in the activated sludge flocs [2]. Different set ups were employed to measure parameters including temperature, pH, solution conductivity and DO concentration. Additionally, photometric methods were utilized to measure concentrations of ammonia, nitrate, nitrite, total nitrogen, total phosphorus and chemical oxygen demand. The measured DO concentration in the bioreactor was approximately 0.2 mg/l. This concentration favored the denitrification process, but was too low to facilitate complete nitrification. Obtained results demonstrated an effective wastewater treatment (ranging from 72 to 80%) for nitrogen compounds removal. A notable reduction in the concentration of nitrites and nitrates in the treated water indicates that the denitrification process was very successful. However, ammonia nitrogen and total nitrogen concentrations in effluent remained high, which induce demand for further improvements. Results showed inhibited nitrification efficiency due to suboptimal DO levels. Establishing the right DO concentration is crucial for successful treatment [3]. Further optimization is needed to achieve satisfactory nitrogen compound removal and meet emission standards.

Acknowledgements

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PY-EnvTech-07

Electrochemical recovery of chromium from tannery industrial wastewater

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Introduction

Chromium is considered an essential raw material for the development and production of key technologies for the transition to a green economy. Since Spain lacks significant chromite deposits, its industry relies on imports of this metal. An alternative source of chromium supply can be found in industrial wastewaters, which contain high concentrations of chromium (≥ 500 ppm). In addition, Cr(VI) is one of the most harmful pollutants often found in wastewater, being a serious health and environmental problem. By means of an appropriate treatment, it would be possible to recover chromium from the industrial wastewater, allowing it to be reused as a high-quality secondary raw material while also minimizing water pollution. In this work, the recovery of high value-added chromium from highly concentrated tannery industrial wastewaters is studied by using cathodic treatments [1,2].

The experiments have been carried out in a discontinuous stirred tank electrochemical reactor at room temperature. The effects of the initial Cr (VI) concentration, the nature of the electrodes, and the treatment time have been investigated to optimize the conditions for maximizing chromium recovery. For this purpose, the concentration of Cr (VI) (UV-vis- spectroscopy) and other metals (ICP-MS) and parameters such as total organic carbon (TOC), chemical oxygen demand (COD), pH, conductivity, in the wastewater have been measured at different times during the electrolytic treatments. In parallel, cyclic voltammetry has been used to study the electrochemical reactions of chromium on the different electrodes and under the different conditions.

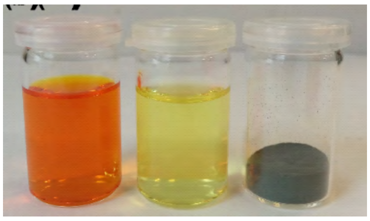

Figure 1. Pictures of the tannery industrial wastewater before (a) and after (b) 3h of electrochemical treatment; and of the precipitate (c) resulting from the treatment.

The obtained results (see Figure 1) show that, under certain electrochemical conditions, chromium can be effectively recovered as a solid product from the studied industrial wastewater.

Acknowledgements

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PY-EnvTech-08

Effective PFOA electrochemical removal from water using a $Ti/SnO_2–Sb/PbO_2$ electrode

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Introduction

Perfluoroalkyl substances (PFAS) pose a global significant threat to water quality due to its stability and wide use. Although there are available some remediation PFOA techniques, there is still more to be learned about the exposure, monitoring and removing of PFAS. Their remediation techniques need to be strong enough to decompose C-F bond, but cost-effective enough to ensure its possibility to be applied [1].

In this study, perfluorooctanoic acid (PFOA) served as a model compound represented a broader class of harmful per- and polyfluorinated substances, while an electrochemical oxidation was chosen as a removal technique [2]. A cerium-enhanced $Ti/SnO_2–Sb/PbO_2$ electrode was developed and selected as a novel approach for PFOA electrochemical removal. Moreover, a custom-built 3D-printed reactor was employed to eliminate potential glass interactions and ensure a constant electrode distance.

To optimize the process, a Box-Behnken experimental design was employed to evaluate the effects of current density, initial PFOA concentration, and supporting electrolyte concentration (Na_2SO_4) on PFOA removal. Fluoride ion release was monitored using a fluoride-ion-selective electrode to assess PFOA degradation. The degradation efficiency was expressed in the defluorination rate.

The $Ti/SnO_2–Sb/PbO_2$-Ce electrode showed enhanced stability and lower energy consumption compared to $Ti/SnO_2–Sb/PbO_2$ and $Ti/SnO_2–Sb$, under identical treatment conditions. Results demonstrated that increased current density positively correlated with defluorination rate, while the initial PFOA had a negligible effect. Under optimal conditions, over 15% of defluorination rate was achieved within 2 hours at a current density of 45 mA/cm^2 with PFOA initial concentration 0.17 $mmol/dm^3$. Moreover, no significant pH drop and voltage change was observed.

This study highlights the potential of Ce-enhanced electrochemical oxidation as a promising technology for PFOA remediation, contributing to the development of sustainable water treatment solutions.

Acknowledgements

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PY-EnvTech-09

Hypochlorite activation by spinel ferrites for sulfonamide degradation: Mechanistic insights for potential application in wastewater treatment

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Introduction

In recent years, applications of hypochlorite has shown potential use in treating wastewaters [1,2]. Besides the activation of HOCl by UV, transition metals can be also used to improve the oxidation efficiency and achieve complete mineralization of organic pollutants. According to the literature, the identification of reactive species (radical or non-radical) generated during activation as well as activated surface complexes has not been elucidated yet. The goal of this work is to provide insights into potential activation mechanism of HOCl using spinel ferrites ($NiFe_2O_4$) focusing on both mechanism and efficiency toward Sulfamethizole degradation in water.

In the current study, $NiFe_2O_4$ was combined to HOCl shown a synergistic due to the participation of metal ions redox and photocatalycal properties of catalyst. The activation mechanism of hypochlorite in accessing the role and contribution of reactive species has been determined using advanced spectroscopic techniques such as XPS and EPR along with chemical scavenging experiments. In addition, the degradation products have been analyzed by LC-MS and the system has been tested in different water matrices (e.g., sewage treatment plant water and tap water) to highlight the applicability of our findings. Thereby, using transition metal ferrites to activate hypochlorite may be an efficient method to incorporate in WWTPs.

Acknowledgments

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PY-EnvTech-10

Enhanced copper selectivity in multi-element solutions using thiourea formaldehyde-functionalized graphene oxide

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Introduction

Due to its high electrical conductivity and durability, copper (Cu) is crucial for renewable technologies, particularly in wind energy. Wind turbines rely on Cu for power generation, transmission, and control systems. Considering an average output of about 3 megawatts (MW) per industrial onshore wind turbine, it can be estimated that there are currently around 270,000 wind turbines in operation worldwide [1]. Additionally, onshore wind farms require 3.9 tons of Cu per MW, while offshore wind farms need 10.5 tons of Cu per MW [2]. As a critical raw material, Cu is vital to the growing demand for renewable energy, but its limited supply and increasing demand make efficient resource management crucial [3]. Although Cu was considered a potentially toxic metal and its removal from waters have been extensively evaluated, its recovery from end-of-life wind turbines is poorly evaluated. On one hand several adsorbents have been studied for the removal of Cu from solution, on the other the studies were conducted in mono-element assays and when considered a complex scenario, only the interaction with potentially toxic elements (i.e., Cd, Pb, Ni, As, and Hg) was evaluated [4]. Recycling technologies have already evolved from primitive methods to more sophisticated techniques such as automatic disassembly and chemical leaching, however the selective separation and recovery of complex mixtures remains a challenge. Therefore, it is important to reduce the dependence on primary mining and its environmental impact, also supporting a circular economy.

The present work aims to evaluate the ability of thiourea formaldehyde graphene oxide (G3DTF) to selective remove Cu from complex mixtures simulating a permanent magnet from a wind turbine waste leachate.

The evaluated mixture simulated the composition of the nacelle component (Cu, B, Ni, Co, Nd, Dy, Pr, Y, Tb) in different concentrations (100 µg/L, 100 µM and real concentration diluted 10-fold). The results showed that G3DTF was selective for Cu after 24 h (removal of 91, 82 and 68 % with increasing concentration) with negligible removal of the remaining elements (2–15 %). Optimization of Cu removal was performed using the response surface methodology. The factors studied were: sorbent dosage (0.2, 1.1, and 2 g L^{-1}), salinity (0, 15, and 25), and pH (4, 6, and 8). The results showed that the sorbent dosage was the most important factor, while salinity and pH were not found to be significant for the removal process of Cu by G3DTF in a multi-element solution.

Overall, the results support the use of graphene-based materials as alternative sorbents to efficiently recover Cu from complex mixtures.

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PY-EnvTech-11

Novel photocatalyst for advanced photocatalytical degradation of methyl orange

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Introduction

A significant reduction in environmental quality inevitably affects global health. Traces of various organic molecules have been detected in all spheres of life, raising concerns about the continued functioning and survival of various plant and animal species [1]. Wastewater, with all its constituents, has a negative impact when discharged into a recipient without prior treatment. Different techniques were utilized for water purification, while advanced oxidation techniques gave the best solutions [2]. The aim of this work is to examine the efficiency of the newly synthesized photocatalyst $Y\text{-}TiO_2$ for the degradation of methyl orange (MO) dye in aquatic environments. The fabricated catalyst was subjected to structural and morphological investigations. During the photocatalytic tests, process parameters such as pollutant concentration, catalyst mass, radiation source distance, and added hydrogen peroxide (HP) concentration are varied. The best results were obtained at a dye concentration of 10 ppm in a system with 0.10 g of catalyst. With the addition of HP at a concentration of 0.015 mg/l, the time required for complete dye degradation was 45 min, compared to 65 min in the system without HP. The analytical measurements of the degradation process was monitored by UV/Vis spectroscopy, and the calculated efficiency was 95%. The obtained results show the great power of the synthesized photocatalyst to decompose the anionic dye under the influence of simulated solar radiation.

Acknowledgements

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PY-EnvTech-12

Optimization of aqueous phenols sorption in by biomass of African breadfruit

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Introduction

The extensive utilization of phenols and its congeners and their uncontrolled release in various manufacturing processes makes them pervasive in industrial wastes and poses a major threat to surface and ground waters [1]. To mitigate this environmental damage, the application of optimized methods of removal in large scale processes is imperative. Herein, the optimization and sorption characteristics of phenol and its congeners in aqueous solution by *Treculia africana* Hull powder (ABHP) [2,3] was investigated under various operating variables such as pH, biosorbent dose (BD), contact time (CT), initial contaminant concentration (ICC) and temperature at 30 °C, 35 °C and 40°C. Optimum sorption over ABHP was reached at pH 6, BD of 1.0 g, in 20 min contact time. Kinetic studies were consistent with a non-linear regression, suggesting a pseudo first order reaction. Among the Langmuir, Freundlich and Sips isotherm models, the latter (Sips) was more consistent with considerable coefficient of determination (~0.97). The FTIR spectra of ABHP clearly revealed the roles of carboxylic acid (C-O), carbonyl (C=O), nitrile (C≡N), amine (N-H) and halo compound (C-Br) in the activity of ABHP. The process was thermodynamically favorable, exothermic, and spontaneous. Based on the bacteria's 16S conserved region, the sequence BLAST prediction report showed that a soil isolate (AIS 2) from a pharmaceutical industry was 99% identical to *Serratia marcescens,* accession number KU522248.1. *Serratia marcescens* immobilization on African breadfruit hull powder, however, improved the removal of phenol and its' congeners, suggesting their potential use in activated sludge processes to remove phenols from industrial wastewater effluents.

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P-GreenChem-01

Application of ICP-MS for assessing bioaccessibility of metals from food supplements

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Introduction

Food supplements are considered as concentrated source of vitamins and minerals that are intended to correct nutritional deficiencies, maintain an adequate intake of certain nutrients, or to support specific physiological functions. Hence, and in order to stablish their nutritional and physiological effects, they became a regular part of our daily diet. The health effect of the supplements depends on various factors as one of them is the fraction of nutrients that are available for subsequent assimilation. Therefore, in the last few years, many studies have been devoted to the assessment so-called *bioaccessibility* of some micro- and macro elements (i.e., Zn, Cr, Fe, Se, Ca Mg, among others) from food and food supplements.

The term *bioaccessibility* refers to the amounts of different compounds that are released from the matrix into the digestive tract and thus became potentially available for absorption (i.e., available to enter the blood stream of the human body). Among the different in-vitro approaches, physiologically-based extraction test (PBET) is considered as a suitable extraction method for predicting the bioaccessibility of metals from a solid matrix. The PBET is a simulated gastro-intestinal extraction procedure which mimic the effects of the human-digestion process.

In the present work two different PBETs were used for assessing the amount of some macro and micro elements from two oral food supplements. To simulate the gastric juice ~~a~~ pepsin (i.e., a common gastric enzyme) was mixed with different reagents as NaCl, citrate, acetic acid and etc. in media of hydrochloric acid, according to the extraction method. The analyzed samples were mixed with the freshly prepared gastric juice in plastic tubes and stirred for 1 hour at 100 rpm. During the procedure the samples were incubated at 37˚C. In order to evaluate the total concentration of the analyzed elements, both samples were subjected to microwave-assisted acidic digestion. The concentration of the analyzed elements in the obtained supernatants after the PBET extractions, together with the microwave digested samples were determined by ICP-MS. The bioaccessible fraction (%) was calculated as the ratio between the concentration of an element found in the gastric extracts and the total metal concentration in the samples.

Acknowledgements

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P-GreenChem-02

Natural deep eutectic solvent – based dispersive liquid-liquid microextraction of pesticides in drinking water combined with GC-MS/MS

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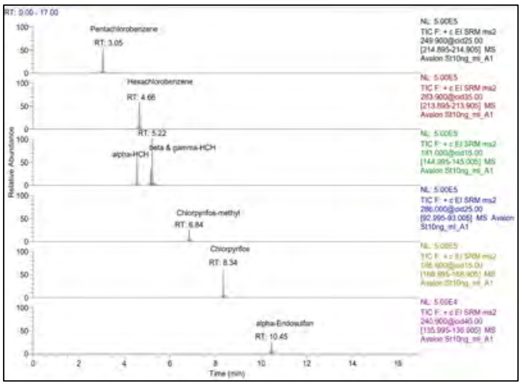
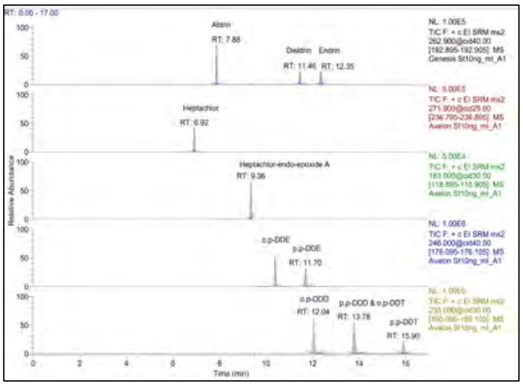
Introduction

The aim of the current study has been to develop a new analytical method applying a dispersive liquid-liquid microextraction assisted by vortex using an environmentally friendly extractant for the preconcentration of 19 organochlorine and organophosphorus pesticides followed by gas chromatography-tandem mass spectrometry (GC-MS/MS) analysis. The extractant has been a natural deep eutectic solvent (NADES) (i.e., safe, cheap and biodegradable) prepared by simple mixing of DL-menthol and decanoic acid (molar ratio 2:1). A number of experimental factors such as (i) sample volume; (ii) NADES volume; (iii) sample pH; (iv) extraction time; (v) centrifugation time; (vi) centrifugation speed; and (vii) ionic strength (NaCl %, w v^{-1}) have been assessed for significance and have also been optimized. A two-step multivariate approach has been employed, comprising a Plackett-Burman design followed by a central composite design (CCD). The sample and the NADES volumes have been distinguished as significant variables, whose optimal values are 10 mL and 45 µL, respectively. The remaining factors have been set at 3 min extraction time, 5 min centrifugation time and 900 x g centrifugation speed. No pH adjustment as well as addition of NaCl have been needed. Under the optimised extraction conditions, the obtained limits of quantification (LOQs) ranged between 0.2 and 78 ng L^{-1} for the studied pesticides. Furthermore, the proposed analytical method has been successfully applied to bottled spring water samples from Bulgaria. A recovery study (n=3) has been proceeded by spiking the samples at three levels (i.e., 0.1, 1.0 and 5.0 µg L^{-1}) and the obtained recovery values and RSD values have been ranged between 70 % - 117 % and 1 % - 20 %, respectively, for all target analytes, except for p,p-DDT (recovery values 56 % - 77 % in high conductivity water samples).





Acknowledgements

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P-GreenChem-03

Development of a sustainable solution based on biopolymer bottles for water sampling in quality control laboratories

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Introduction

Controlling the quality of drinking water is a fundamental aspect of public health, as ensuring the best possible water supply is a guarantee of a healthy population. To achieve this, quality control laboratories play an essential role in the prevention and control of potential risks associated with water contamination issues [1]. This involves the collection of samples for subsequent transfer to the designated facilities for analysis [2].

Conversely, the excessive use of plastics (non-biodegradable polymers) for water collection leads to the emergence of a new form of contamination, as the polymers used in their manufacture do not degrade. Plastics degrade in three ways: mechanically, chemically or by photodegradation, resulting in the formation of microplastics (MP) and nanoplastics (NP).

In drinking water quality control laboratories, a large number of non-biodegradable polymer bottles are used for sampling. This source of contamination is contrary to the principles of green chemistry or environmentally friendly chemistry, which states that quality control laboratories must not introduce a new type of contamination that jeopardises the quality of the product under analysis. Accordingly, the use of bio-based, biodegradable or compostable bottles can be an alternative to the various containers currently used for sample collection in quality control laboratories [3].

Preliminary results show that polylactic acid (PLA)-based polymers are a promising alternative material that contributes to the reduction of the carbon footprint.

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P-GreenChem-04

Influence of PFAS on the cucumber (*Cucumis sativus*): antioxidative enzymatic response

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Introduction

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental pollutants with significant implications for ecological and human health due to their resistance to degradation [1]. The accumulation of PFAS in plants presents a risk to the food chain, but on the other side an opportunity for phytoremediation. Understanding the interaction between PFAS and plant systems is crucial for assessing the risks and exploring the potential of phytoremediation. To date it is well known that PFAS cause numerous perturbances in plant's biological activities including the over-generation of reactive oxygen species (ROS). Increase of ROS triggers an enhanced activity of antioxidant enzymes in plants exposed to PFAS [2]. However, in cucumber (*Cucumis sativus*), one of frequently examined PFAS contaminated vegetable [3], the most effective antioxidant enzyme activities- superoxide dismutase (SOD), catalase (CAT), as well as oxidase laccase, as an indicator of oxidative stress response, have not been determined, to date.

The aim of this study was to investigate the cucumber antioxidant response to presence of high concentration of PFAS: perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS), studying the activity of SOD, CAT and, particularly, laccase whose potential to participate in degradation of PFOA was indicated [4].

In plants exposed to PFOA, SOD activities increased by 43% and 52% in aerial part of plants and roots, respectively, while in plants exposed to PFOS, SOD activities increased by 45% and 64% in aerial part of plants and roots, respectively. Catalase activity in the roots of plants exposed to PFOA and PFOS, compared to the control, was significantly increased: 10- and 8-fold, respectively. No laccase activity was detected in control plant, while exposure to PFAS, both PFOA and PFOS, strongly induced laccase activity in roots.

Cucumber exposure to PFAS causes increased activity of antioxidant enzymes SOD and CAT comparing to control samples, indicating an enhanced ROS production as a result of altered redox homeostasis. More importantly, laccase activity initiated in PFAS treated cucumber, suggesting not only plant response to oxidative stress damage, but as well its potential role in the removal process of PFAS. For a deeper insight into the mechanism of response of plants to PFAS exposure, a comparative proteomic analysis is underway.

Acknowledgements

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P-GreenChem-05

Recent advances in supercritical extraction from grape pomace for a sustainable biorefinery in the wine industry

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Introduction

The research presents a pioneering investigation into the supercritical carbon dioxide (SC-CO2) extraction of policosanol (PC) from grape marc, representing the first exploration of its kind. Utilizing the broken plus intact cells (BIC) model (Sovova's model), the efficacy of SC-CO_2 in extracting the nonpolar fraction from grape marc is scrutinized. Optimal operating conditions—280 bar pressure, 70°C temperature, and a flow rate of 10 kgCO_2/h—yielded the highest policosanol content. Policosanol levels ranged from 3922 to 4083 mg/kg_{DM}, comprising approximately 8% of the total extraction yield. Surprisingly, this policosanol quantity matches that found in beeswax yellow, a renowned natural PC source. The primary aliphatic alcohols identified in grape marc PC were hexacosanol, octacosanol, and triacontanol, consistent with samples from other Italian regions.

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P-GreenChem-06

Ligandless dispersive liquid-liquid extraction of lanthanides with NADES

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Introduction

Natural deep eutectic solvents (NADES) are comparatively new media used as a green alternative to classical solvents. They are recently preferred by many researchers because of their properties as low or no toxicity, low price, bioavailability and biodegradability. Besides this, NADES have negligible volatility and high capacity for dissolution of variety of chemical compounds. For these reasons natural deep eutectic solvents have found their application for extraction of various organic and non-organic analytes.

In the current investigation, a procedure for ligandless dispersive liquid-liquid extraction of lanthanides (i.e La, Ce, Eu, Er, Gd, and Lu) with natural deep eutectic solvent is studied. The extractant is synthesized from DL-menthol and decanoic acid in molar ration 2:1 according to procedure described in [1]. Parameters of the extraction system as sample pH, extraction time and volume of NADES are optimized. It was found that lanthanides are quantitatively extracted in neutral and basic media in 100 µL of the solvent in less than a minute. The hydrophobic phase is separated from the sample solution after refrigeration. Analytes are then recovered in 0.1 mol L^{-1} nitric acid and measured by microwave plasma – atomic emission spectrometry (MP-AES). Recoveries above 80% are achieved for all target analytes.

The presented extraction method of lanthanides from aqueous samples is green, fast and simple.

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P-GreenChem-07

Earth-abundant carbon-based catalysts for visible light-driven H_2 evolution from water

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Introduction

The industrialization and constant increase of population have drastically contributed to the worldwide energy shortage and environmental pollution issues. The use of renewable energy resources, such as solar light, has emerged as an attractive and sustainable substitute to produce green energy and mitigate the shortage of fossil fuels. In this context, photocatalytic water splitting is regarded as an environmentally friendly technology to produce solar fuels such as H_2 from sunlight energy and water in the presence of a photocatalyst [1]. Furthermore, the activation of the photocatalytic reaction requires the loading of metallic co-catalysts onto the surface of the photocatalyst. The co-catalysts are often metallic nanoparticles (NPs), such as Pt, that promote charge separation of photogenerated electrons and holes and work as active sites for the catalytic reaction [2].

Polymeric carbon nitride, g-C_3N_4 (GCN), a metal-free semiconductor mainly composed of carbon and nitrogen atoms connected via tri-*s*-triazine units (Fig. 1), was firstly tested for visible light H_2 evolution in 2009 [3]. It presents unique features such as response in the visible region of the solar spectrum (E_{bg} = 2.7 eV), low toxicity, low cost and high chemical stability, among other properties. Nevertheless, bulk GCN presents as main drawbacks low surface area, limited absorption in the visible region and high recombination of charge carriers (electrons/holes), resulting in low photocatalytic activity. In this context, several strategies have been employed to overcome these limitations, such as thermal and chemical exfoliation, functionalization with other nanomaterials (TiO_2, graphene, etc.), metal and non-metal doping, etc. [4].

In the current work we intend to discuss how the modifications performed to bulk GCN (exfoliation and doping), as well as the type of co-catalyst employed (Ni and Cu NPs), influence the photocatalytic performance towards H_2 evolution under simulated solar light (Xe lamp; TEOA 10% V/V). The Ni and Cu NPs were prepared using the organometallic approach [5], which allows to obtain monodisperse metallic NPs of narrow size distribution and a controllable size and surface environment. Furthermore, all the materials were characterized by several techniques (XRD, photoluminescence, DRS UV-vis, TEM, FTIR, XPS, ICP, electrochemistry) allowing to obtain a correlation between GCN structure and activity, adding valuable insights to the continuous research on green solar fuels over carbon-based nanomaterials.

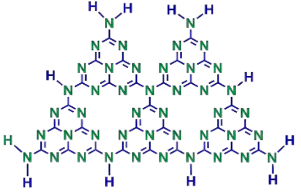

Figure 1. Heptazine (tri-*s*-triazine) structure of g-C_3N_4 (GCN).

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P-GreenChem-08

CO_2 conversion: unraveling the effect of hydrophobicity, porosity, and functionalization of nanoporous activated carbon based electrodes

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Introduction

The electrochemical reduction of CO_2 (CO2ER) in aqueous or gas phase is an alternative to mitigate the environmental impact generated by massive CO_2 emissions, in addition to forming value-added products like carbon monoxide (CO), formic acid or ethanol, to cite just a few of them. In this sense, numerous reported publications are devoted to the search for electrocatalytic materials other than those based on metal electrocatalysts, e.g. nanoporous carbon materials [1]. Their electrocatalytic activity for CO2ER is studied by electrolysis in electrochemical cells, where the cathode is the nanoporous carbon material coated on a conductive inert support [2], where Toray carbon paper (TCP) is one of the most widely used. In this work, the effect of the percentage of PTFE coating on the TCP support (0, 5 and 20%) for nanoporous carbon-based electrodes (coated by aerography with ink: 75/25 wt.% carbon/Nafion in ethanol,) for the CO2ER performance has been firstly evaluated using a commercial nanoporous carbon with control of the microporosity and surface chemistry functionalization. CO2ER electrolysis performed at controlled potential during 6 h using a 0.5 M $KHCO_3$ solution saturated with CO_2 solution reveal that the presence of PTFE on the TCP support reduces both the H_2 and CO generation, obtaining the highest selectivity of CO for the nanoporous carbon based electrodes onto the TCP containing 5% of PTFE. The highest production rate of CO of the TPC series was obtained when performed CO2ER in the absence of PTFE. Secondly, the role of porosity has been less addressed, consequently, this work also explores the electrocatalytic activity of CO2ER of a series of four nanoporous carbon materials with different amount of microporosity volume, average pore size and their control of mesoporosity (physical overactivation processes of a commercial microporous carbon material with CO_2 at 775 °C for 4, 8 and 16 h). The results reveal an effect of the porosity of the carbon material on the selectivity and faradaic efficiencies on the CO production with increasing pore volume, the average pore size and the development of mesoporosity, which electrochemical indicators may be associated with the interaction and nano-confinement of CO_2 molecules and reaction intermediates present in the nanoporosity of the electrode. Thirdly and finally, with regard to the surface chemistry of the nanoporous carbon, a high amount of O-content present in the nanoporous carbon is detrimental for the CO2ER when keeping constant the same microporosity, and the CO2ER performance is independent of the electrode potential applied to the electrolysis. Moreover, a temperature programme decomposition of the aforementioned carbon results in the control of the surface chemistry e.g., carboxylic, anhydride, lactone, phenols and quinone groups, respectively, dictating the production and selectivity of CO.

Acknowledgements

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P-GreenChem-09

Circular economy applied to nitrate removal: hydrogen generation and waste recovery in drinking water (LIFE ELEKTRA)

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Introduction

Nitrate pollution in surface and groundwater affects many member states of the European Union. An excess of nitrate in water is harmful to human health and for the ecosystems and, consequently, its elimination is a priority. In October 2023, a LIFE project was started whose name corresponds to the title of this communication. The project focuses on the validation of the electrochemical denitrification technology applied to the treatment of water with high nitrate concentration, by transforming nitrate into nitrogen gas that is emitted into the atmosphere without impacting the environment [1]. The partners that make up the consortium are: *Aguas de Valencia S.A.*, *Universidad de Alicante*, *Asociación Instituto Tecnológico de la Energía*, *Universitat de Valencia*, *Apria Systems S.L.*, *Instituto Tecnológico de Canarias*, *Water Services Corporation WSC* and *Redinn SRL*. The project addresses three case studies, located in Spain (Valencia and the Canary Islands) and the Republic of Malta, each one of them with different characteristics, but with the same challenge to give solution for nitrate pollution in different types of water. A mobile pilot plant is being designed and will be built by coupling a renewable energy hybridization system to cover the electrical energy needs of the process. In this way, the high transferability of the proposed solutions will be demonstrated, allowing the removal of nitrates in a sustainable and energy-cost effective way. The Applied Electrochemistry and Electrocatalysis Group at the University of Alicante plays a relevant role in the development of the project since it is the owner of the electrochemical denitrification technology [2] that is incorporated in the prototype that is already being developed. Results will be presented in terms of the electrochemical treatment of real waters from the rejection of a well water purification plant by means of reverse electrodialysis (EDR) and with nitrate contents ranging between 400 and 1600 ppm. The electrochemical conversion of real water containing nitrate produces H_2 and N_2 as main products in gas phase and NH_4^+ ion as a minor subproduct in solution, with no other gaseous species like NO_x. This gaseous mixture which is fundamentally made up of H_2 with a percentage of N_2 lower than 3% is subsequently used as a feed gas for a fuel cell in order to recover part of the electrical energy supplied.

Acknowledgements

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P-GreenChem-10

Analysis of fragrance allergens in cosmetic products using GDME-GC-MS/MS

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Introduction

Gas Diffusion Microextraction (GDME) is an extraction technique in which analytes are separated from the sample by diffusion into a small volume of acceptor solution supported by a microporous membrane that is permeable to gas but not to liquid. This technique is based on the diffusion of analytes so, it is applied to volatile and semi-volatile compounds [1,2].

For the first time, an analytical methodology based on GDME followed by gas chromatography coupled to tandem mass spectrometry (GC-MS/MS) is proposed for the determination of allergenic fragrances in aqueous and alcoholic-based cosmetic products. The experimental extraction conditions were optimized through an experimental design that evaluated the influence of six parameters: acceptor solution volume, percentage of acetonitrile in the acceptor solvent, sample dilution, salting-out effect, extraction time, and sample volume. Under optimized conditions, the method was validated in terms of linearity, precision, and accuracy, showing satisfactory results. Finally, the validated methodology was applied to 12 real samples of cosmetic products, in which 11 of the 12 samples contained the studied allergenic fragrances, demonstrating the widespread use of these compounds in personal care products. These substances are considered emerging contaminants in the environment, mainly reaching it through urban waters.

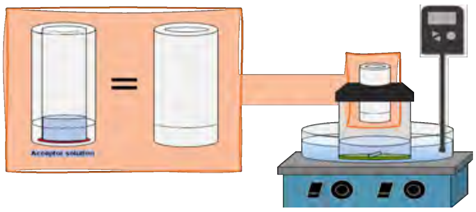

Figure. Scheme of the GDME procedure.

Acknowledgements

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P-GreenChem-11

Highly selective biomass-derived catalysts for the conversion of Levulinic Acid to Gamma-Valerolactone

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Introduction

Gamma-Valerolactone (GVL) is proposed to be one of the top 12 platform chemicals by the US Department of Energy, since it is a versatile molecule that can be used as a fuel additive, food additive, and intermediate for the synthesis of chemicals and solvents [1]. GVL can be obtained from the hydrogenation of levulinic acid (LA), which in turn can be achieved from lignocellulosic biomass. Several approaches have been considered to convert LA into GVL, which include the selection of catalysts with various compositions, both noble metals (i.e. Ru, Pd, Au), and non-noble metals (i.e. Cu, Ni, Fe, etc.) [2, 3], and cover different experimental conditions that normally involve harsh reaction conditions such as high temperature and high hydrogen pressure. The present study addresses a facile and eco-friendly approach to synthesise GVL from LA using biomass-derived carbon-supported Ru catalysts and using mild reaction conditions.

Biomass-derived activated carbons were obtained from lignocellulosic biomass residues, namely hemp residue (HR) and almond shell (AS), by a H_3PO_4-assisted hydrothermal carbonisation (HTC) [4]. The synthesis was performed by mixing 1 g of HR or 2 g of AS with a low concentration aqueous solution of H_3PO_4 (25 wt %) in a 50 mL Teflon-lined stainless-steel autoclave (weight ratio of H_3PO_4/HR equal to 1 and H_3PO_4/AS equal to 2). The autoclave was heated at 200 °C for 24 h. The resulting hydrochars were heated at 450 °C for 2 h in a N_2 atmosphere (50 mL min^{-1}). The obtained activated carbons were washed with distilled water at 65 °C and dried at 110 °C overnight. Ru catalysts were synthesised from the developed biomass-derived supports using a standard impregnation method followed by reduction with $NaBH_4$. The catalysts were analysed by means of several characterisation techniques such N_2 adsorption-desorption experiments, TEM, ICP, XPS, etc. The conversion of LA to GVL was carried out in a pressurised 100 mL stainless steel batch reactor using 100 mg of catalyst, 0.5 g of LA and 25 mL of distilled water. The reaction was performed at 70 °C for 1 h with a hydrogen pressure of 15 bar.

The characterisation of the catalysts indicated that they have a very low Ru loading (~ 0.5 wt %) in the form of small and well-dispersed nanoparticles. Both metallic and oxidised Ru species were detected in the fresh catalysts. The analysis of the reaction products revealed that the developed catalysts displayed excellent results in terms of both conversion of LA and selectivity to GVL, as well as great catalytic stability. This study highlights the potential of attaining an overall sustainable process that encloses the utilisation of biomass-derived catalysts for the conversion of LA to GVL. Furthermore, it can serve as a platform to convert LA into other countless valuable chemicals using biological feedstocks in integrated biorefineries.

Acknowledgements

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P-GreenChem-12

Phytoremediation of water polluted with perfluorooctanoic acid and perfluorooctanesulfonic acid

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Introduction

Due to their unique hydrophobic and lipophobic properties and long-term usage for various applications in industrial and consumer products, the environment has been extensively contaminated by per- and polyfluoroalkyl substances (PFAS) [1]. Exposure to PFAS may lead to various health issues, including reduced fertility, developmental delays in children, increased cancer risk, weakened immune system, higher cholesterol, and obesity [2]. Long-chain perfluorocarboxylic acids (PFCA), such as perfluorooctanoic acid (PFOA) are highly persistent, bioaccumulative, and toxic. Long-chain perfluorosulfonic acids (PFSA) such as perfluorooctanesulfonic acid (PFOS) bioaccumulate less in animals but readily translocate in the leaves and stems of plants. However, their occurrence, behavior, fate, and toxicity are poorly understood. The chemical composition and behavior of PFAS make them difficult to remove from the environment using traditional physical or chemical treatments. Various techniques such as adsorption, photocatalysis, electrochemical oxidation, thermolysis, and biological treatment are being used for effective PFAS remediation. However, these methods often require a lot of energy and come with high operating costs. Phytoremediation utilizes natural processes to clean up soil and water contaminated with PFAS. This approach uses plants to absorb and disperse PFAS within their structures, making it a promising technology. Our study aimed to study the phytoremediation as a mechanism for PFAS removal. Plants (*Cucurbita pepo L.*) were grown hydroponically in the presence of high concentrations of PFOA or PFOS (0.1 mg/L) using the germination test, and further investigated their potential to degrade them. The effects of PFAS on plant growth were monitored by measuring the length of the plant's roots and stems. Additionally, a SpectraVue Leaf Spectrometer was used to obtain leaf spectra in the range of 330-1100 nm and to determine Normalized Difference Vegetation Index (NDVI). The accumulation of PFOA and PFOS in plants was monitored using target HPLC analysis and enzymatically by detection of superoxide dismutase activity. Chemical and biochemical analysis showed enhanced activities of superoxide dismutase in leaves and stems, and roots, as well as a slight increase in spectral characteristics of leaves at A670 nm in plant growth in water with PFOA and PFOS compared to the control water sample. The NDVI of the leaves in hydroponic plants with PFOA and PFOS showed a slight decrease compared to control plant leaves. Phytoremediation has the potential to be a cost-effective, long-term solution and can be widely implemented as an *in situ* remediation strategy. However, future studies will confirm whether the phytoremediation is a suitable method (and in which cases) for the treatment of PFAS polluted water bodies.

Acknowledgements

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P-GreenChem-13

Green synthesis of selenium nanoparticles using cationic cellulose nanofiber and chitosan for active food packaging application

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Introduction

There is a growing interest in the synthesis of nanoscale metals using chemical, physical and green synthesis. However, physical and chemical methods are gradually replaced by the green synthesis approaches due to concerns about the high energy consumption, the release of toxic chemicals and the need for complex equipment and synthesis conditions showed by the formers [1]. Green synthesis offers economical, environmentally friendly and more sustainable way of synthesis strategies. Traditional single-variable optimization methods overlook the interaction between variables leading to incomplete results and higher costs. Here comes the role of response Surface Methodology (RSM), which addresses this by using a statistical and mathematical technique to fit polynomial methods to data [2].

This research deals with the novel synthesis of spherical selenium nanoparticles (Se NPs) using sustainable and biocompatible agents like cationic cellulose nanofibers (CCNF) or chitosan (CS) as stabilizers and their optimization using RSM methodology. Sodium selenite (Na_2SeO_3) and ascorbic acid are used as the metal precursor and reducing agent, respectively. RSM model was designed using different concentrations of Na_2SeO_3, ascorbic acid and CCNF or CS as three independent variables with size and stability as response factors. The R^2 value was found to be close to 1 indicating that the model generated was statistically significant. From the combined contour plots of the RSM model, CS-Se NPs of size and zeta potential 10-70 nm and 30-40 mV, respectively, were synthesized when the concentration of Na_2SeO_3 and ascorbic acid were 0.7 M and 1.8 %wt of CS. While in the case of CCNF-Se NPs, size and zeta potential of 50-85 nm and 30-35 mV, respectively, were synthesized when the concentration of the precursor, reducing agent, and CCNF were 0.3 M, 0.5 M, and 0.3 %wt respectively. The synthesized Se NPs were characterized using FTIR, EDX, XRD which of them all confirmed the formation of elemental selenium. FESEM images confirm the spherical size of the Se NPs synthesized by the two different stabilizers. The synthesized CS-Se NPs and CCNF-Se NPs were then incorporated with TEMPO mediated oxidized cellulose nanofibers (CNF) by two incorporation strategies like in-situ and blending. This was then coated on the paper (liner) to be used for food packaging applications. Two layers of Se NP incorporated CNF along with one layer each of polyvinyl alcohol (PVA) and alginate was coated on the paper to improve its barrier properties against water vapor and air. Characterization techniques like water vapor transmission rate (WVTR) and migration test were conducted. The papers showed no significant release into the food simulant and the in-situ synthesized Se NP coated paper showed a lower WVTR compared to the blended and the uncoated ones. The antioxidant property of the Se NP coated paper was tested in the DPPH assay, and it showed an improved antioxidant property.

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P-GreenChem-14

Plasmonic materials for green hydrogen production from water splitting reaction

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Introduction

Fossil fuels are the main responsible for the anthropogenic emission of greenhouse gases, which are linked to the climate change. The search for renewable and clean energy vectors is mandatory to ensure the worldwide energy supply while minimising the environmental impact of the current fossil fuel-dependent energy supply. Hydrogen (H_2) holds great promise as an energy carrier, but major scientific, technical, and socio-economic challenges remain [1]. There are a wide variety of approaches for H_2 production, such as electrolysis, thermal water splitting, hydrocarbon reforming, and so forth, but these approaches are either costly or rely on fossil fuels [2]. Photocatalytic water splitting has burgeoned as an elegant concept towards the sustainable and green production of H_2, since H_2 and O_2 are released using solar energy and minimising, therefore, the carbon footprint [3].

In this work, we have synthesised several photocatalysts based on both stoichiometric and non-stoichiometric MoO_3 and WO_3, and their performance towards the production of hydrogen from the water splitting was assessed. The synthesis of the photocatalysts was carried out by a hydrothermal route and by calcination at 675 ºC in a tubular furnace with an inert atmosphere [4]. In addition, Cu-containing photocatalysts were also prepared by a standard impregnation method. The as-synthesised materials were characterised by means of physicochemical techniques such as UV-Vis spectroscopy, X-ray Photoelectron Spectroscopy (XPS), X-Ray Diffraction (XRD), and Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-OES). The photocatalytic tests were carried out using different experimental conditions, such as including sacrificial agents, evaluating the effect of reaction time, and light sources, which helped us to find out the optimum conditions. It was observed that the production of hydrogen was strongly dependent on the sacrificial agent used in the reaction, and, among the investigated sacrificial agents, methanol provided the best photocatalytic results. The obtained results indicate that, upon the selection of appropriate experimental conditions, MoO_3 and WO_3-based photocatalysts may be suitable candidates to be used towards the production of green hydrogen from water splitting.

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PY-GreenChem-01

Oxygen reduction reaction electrocatalysts based on Mxenes, graphene and metallic nanoparticles

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Introduction

Metal-air batteries, particularly zinc-air batteries (ZAB), represent a promising solution for energy storage due to their high energy density and low cost. However, they face significant challenges related to the kinetics and overpotential of the oxygen reduction and evolution reactions (ORR and OER) [1]. Moreover, the hydrogen evolution reaction (HER) is of both fundamental and practical interest in the generation of green hydrogen in electrolyzers. Current electrocatalysts still require improvements to reduce their reliance on expensive noble metals [2]. In this context, two-dimensional materials such as MXenes, which include transition metal carbides, carbonitrides and nitrides, emerge as promising candidates. MXenes share a structural similarity with graphene but offer superior advantages in electrochemical energy storage. Additionally, combining them with metal nanoparticles holds the potential to optimize electrocatalysts, addressing key challenges in conversion and energy storage aplications [3].

This study focuses on the preparation of two-dimensional materials by two different methods. The first method involves synthesizing a Ti_3C_2-based material from MAX-phase Ti_3AlC_2 via selective etching with hydrofluoric acid (HF), followed by a sequence of stirring, washing, drying and treatment with dimethyl sulfoxide (DMSO) for delamination. The second method focuses on the preparation of graphene-based anodic and cathodic materials through the electrochemical exfoliation of graphite sheets, starting with sulfuric acid treatment and subsequent electrochemical expansion in an electrochemical cell with separation of compartments. Finally, platinum (Pt) was incorporated on these materials by impregnation.

The results reveal a highly efficient material for electrochemical energy storage: a combination of MXene (Ti_3C_2) with anodic graphene (G. ANOD) and platinum (Pt) achieves a specific capacitance of 196 F/g, markedly outperforming other combinations. In comparison, configurations such as MXene with cathodic graphene (G. CAT) and Pt, MXene with Pt, and MXene without additives show inferior performance, underscoring the superior role of anodic graphene and Pt. Furthermore, this material demonstrates outstanding electrocatalytic activity, especially in the hydrogen evolution reaction, which positions it as a viable alternative for the production of green hydrogen in the field of sustainable technologies. Its high capacitance, together with its efficiency in catalytic processes, suggest that this material could also find applications in supercapacitors, significantly improving the efficiency and capacitance of these devices.

Acknowledgements

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PY-GreenChem-02

Deep eutectic solvents as sustainable mixtures in electrosynthesis

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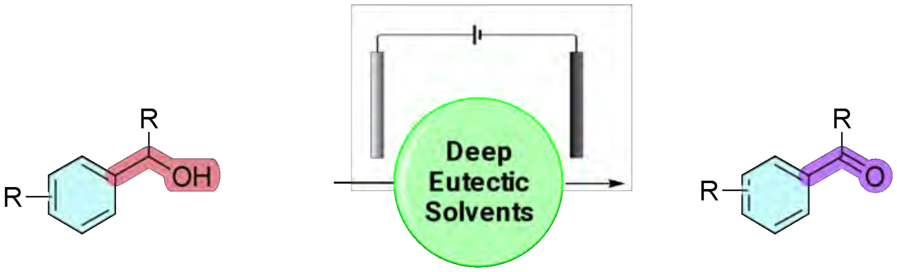
Introduction

Solvents play a crucial role in the synthesis of chemical compound, representing up to 95% of the total mass of a given reaction.[1] Thus, replacing toxic volatile organic solvents is mandatory. In this sense, the use of biorenewable deep eutectic solvents (DESs) have been proposed over the last decade as a sustainable alternative, having already proven hat traditional synthetic procedures can be performed in these neoteric reaction media leading to a dramatical improvement in the overall sustainability of processes.

However, state of the art synthetic methods such as photochemistry or electrochemistry still rely on volatile organic compounds (VOCs) as solvents. Our group already proposed some of the first approaches to photochemistry[2-3] using DES, and herein present a pioneering work regarding organic electrosynthesis in DES, which not only replace the need of use toxic organic solvents, but also the corresponding expensive sacrificial electrolytes.

The oxidation of alcohols to aldehydes and ketones, an important reaction in both fine and bulk chemical industries,[4] has been achieved *via* electrosynthesis using a simple and sustainable eutectic mixture based on magnesium chloride, acetamide and urea.



Scheme 1. Electrochemical oxidation of alcohols in deep eutectic solvents.

Thus, the sustainability and economic viability of the process is greatly improved, since no chemical oxidant is required, while the DES fulfils a double role, *i.e.* as reaction medium and as electrolyte. In addition, the properties and efficiency of various eutectic mixtures have been explored and characterized with the ultimate goal of bringing out the design guidelines for these solvents and, more importantly, to establish the foundations for this emerging research area.[5]

Acknowledgements

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PY-GreenChem-03

Carbon-based supercapacitors with eco-friendly aqueous electrolytes

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Introduction

In response to the urgent need to mitigate climate change, there is a growing focus on reducing society’s dependence on fossil fuels. Although renewable energy sources offer a cleaner alternative, their intermittent nature makes challenging their integration into the electrical grid. To mitigate this intermittency, it is necessary to use energy storage systems such as batteries and electrochemical capacitors or supercapacitors. Supercapacitors stand out for their high-power density, long lifespan, and rapid response to voltage fluctuations. These devices store energy by accumulating charges in the electric double-layer formed between the electrode surface and the electrolyte. Despite their advantages, supercapacitors have a low energy density, which makes it necessary to optimize the electrode materials and operating voltage.

Carbon-based materials, such as activated carbon, are ideal for this purpose due to their high specific surface area and porosity, which facilitate greater charge storage. This research explores the potential of a commercial activated carbon, YP-50F, as an electrode material for supercapacitors. Aiming at enhancing the energy density and overall performance of supercapacitors, this study also evaluates the benefits of both symmetric and asymmetric configurations using an eco-friendly aqueous electrolyte containing Na_2CO_3 which has not been studied in detail in the literature.

The results showed that activated carbon YP-50F exhibits a high apparent surface area and a suitable porous texture for charge storage, with a predominance of micropores. Cyclic voltammetry determined an optimal voltage near 2 V for the carbon material in the aqueous electrolyte Na_2CO_3 0.5M, a remarkably wide voltage window for an aqueous system, which is notable given the typical limitations of such aqueous based electrolytes. Furthermore, the asymmetric supercapacitor outperformed better results than the symmetric configuration in terms of both gravimetric capacitance and stability, maintaining an excellent gravimetric capacitance after 20,000 cycles, such a capacitor performance stands out in comparison with other studies reported for this type of supercapacitors using aqueous-based electrolytes.

Acknowledgements

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PY-GreenChem-04

Exploring Pt-doped CdS/TiO_2 heterostructures for CO_2 photoreduction

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Introduction

The burning of fossil fuels for energy production has led to a growing concentration of greenhouse gases like carbon dioxide in the atmosphere, contributing to global warming and accelerating climate change [1]. To address this environmental issue, photocatalysis using semiconductors has emerged as a promising strategy to convert CO_2 into high added values such as methane. Fujishima and Honda discovered in 1972 that titanium dioxide (TiO_2) could induce the photocatalytic splitting of water when exposed to sunlight. After this breakthrough TiO_2 has become one of the most widely used photocatalysts for environmental applications [2]. Commercially, the most common titanium dioxide used for photocatalysis is P25 (Degussa). P25 presents a crystal size between 20-50 nm, a surface area of approximately 50 m²/g, and a band gap of 3.1 eV. However, P25 has certain drawbacks, including low surface area, limited visible light absorption, and a high rate of electron-hole recombination which prevent it from being a highly efficient photocatalyst in CO_2 photoreduction [3]. The goal of this work focuses on the synthesis of a photocatalyst based on P25 titania and CdS doped with Pt nanoparticles to improve the physicochemical properties of P25. This photocatalyst may form a Z-scheme heterostructure, that improves the charge transfer and the catalytic activity of the heterostructure (Figure 1 (a)) [4]. The CdS, synthesized through a solvothermal method, mainly has a Wurtzite (hexagonal) structure. It is a n-type intrinsic semiconductor with a band gap of around 2.4 eV. On the other hand, the platinum nanoparticles were synthesized from H_2PtCl_6 and a reducing agent using an impregnation method. The materials were characterized XRD, TEM, SEM-EDX, UV-Vis, PL, XPS, UPS and ICP-OES. The obtained results show the successful synthesis of the heterostructure doped with Pt. Moreover, the observed primary function of CdS and Pt nanoparticles is to reduce the electron-hole pair recombination by acting as an electron scavenger, which slows down the recombination process and increases the photocatalyst efficiency by facilitating electron transport at the semiconductor-platinum interface. Thus, Pt-doped CdS/TiO_2 heterostructures with the adequate composition present better catalytic activity than Pt/P25 titania which methane production values are 460 and 397 µmol CH_4/g·h, respectively (Figure 1 (b)).

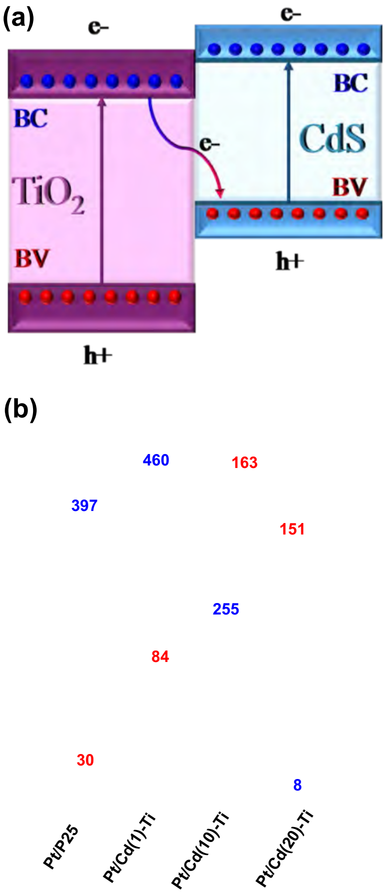

Figure 1: (a) Pt-doped CdS/TiO_2 band structure (b) CH_4 production of the prepared samples.

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PY-GreenChem-05

Exploring Bimetallic Au/Cu Nanoparticles as Immunosensing Platforms

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Introduction

Noble metal nanoparticles have proven to be one of the most important classes of nanomaterials for biosensing. Their importance stems from their unique properties that depend on the size, shape and composition of the nanoparticles. They are also of great interest for important biomedical applications due to their ease of synthesis, characterization, and surface functionalization. Their applications span a wide range of critical biomedical areas, including the detection of proteins and small molecules, identification of disease-specific DNA/RNA sequences, and glucose sensing for diabetes monitoring[1].

Herein, we explore the synthesis, physicochemical and electrochemical characterization of Au/Cu alloy nanoparticles to be used as highly sensitive sensors. The colloids of nanoparticles were synthesized following the reduction-by-solvent method [2], combining both metal precursors during the synthesis process. In this regard, the use of AuCu alloy nanoparticles offers several potential advantages over single-metal nanoparticles, including tuneable properties, enhanced catalytic activity, and synergistic effects between both metals. These characteristics can lead to superior performance in sensing applications, potentially allowing for higher sensitivity and selective detection of biological biomarkers.

Physicochemical characterization is key to determine size, shape, distribution, metal content, presence of functional groups, composition, and oxidation states of surface species. XPS analysis revealed the presence of metallic gold, along with copper in multiple oxidation states: metallic Cu (0), Cu(I), and Cu(II) on the sample surface, with their relative proportions depending on the metal ratio. ICP-OES confirmed the overall metal content, while TEM imaging provided direct observation of the nanoparticles size and morphology. Cyclic voltammetry has been employed to compare the electrochemical behaviour and surface redox activity among the materials. Their corresponding electrochemical surface area has been determined by the integrated charge which can be related to their particle size. In addition, electrochemical activity toward a redox probe (i.e. ferrocene) will help to assess the electrochemical properties and behaviour of electrode surfaces for a subsequent assembly of a label-free immunosensing platform.

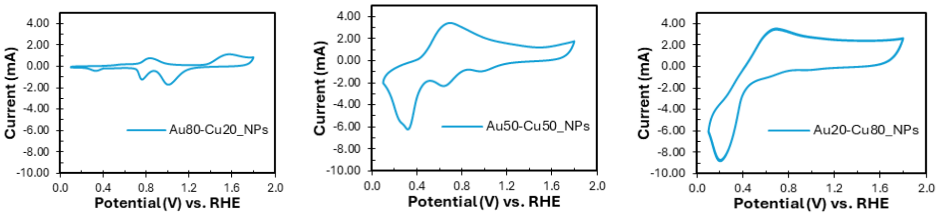

Figure 1. Cyclic voltammograms for different bimetallic of AuCu alloy nanoparticles with different compositions in 0.1 M PBS (Phosphate Buffer Solution, pH 7.2) at 80 mV/s.

Acknowledgements

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PY-GreenChem-06

Effect of temperature on supercapacitors based on activated carbon and neutral aqueous electrolyte

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Introduction

Electrochemical energy storage systems are essential for connecting with renewable energies and reducing dependence on fossil fuels and minimizing greenhouse gas emissions [1]. Electric double-layer supercapacitors or electrochemical capacitors are a promising technology based on the electric double-layer formation on the electrode surface within an electrolyte [2]. Supercapacitors based on activated carbon and aqueous electrolytes at neutral pH are considered the most sustainable and environmentally friendly since biomass-derived activated carbon can be used and it uses a water-based electrolyte [3,4]. Key parameters in supercapacitors, such as ion solvation, ionic conductivity, viscosity, adsorption and diffusion coefficient [5-8], are temperature-dependent, which indirectly affects the final capacitance, energy and power of the device.

In this study, the effect of the temperature on the electrochemical properties of supercapacitors in aqueous electrolyte was evaluated. The preparation of the electrode materials was carried out by mixing a commercial activated carbon YP-50F, acetylene black and Teflon in a weight ratio of 85/10/5, respectively. The electrode material was cut into a 5 mm disc electrode. The activated carbon was dried at 80ºC overnight and a 0.5 M Na_2SO_4 solution was used as the electrolyte. Physicochemical characterization was performed on the commercial activated carbon YP-50F, using nitrogen physisorption at 77 K and temperature-programmed desorption, revealing a specific surface area of 1570 m²/g and a low oxygen content (≈3 % g O/g sample). Electrochemical characterization of the symmetrical electrochemical capacitor was conducted through cyclic voltammetry, chronopotentiometry and electrochemical impedance spectroscopy. The results show that increasing temperature decreases viscosity while increasing ionic conductivity, species diffusivity and capacitance. Also, preliminary results show that thermal energy can be successfully harvested as electrical energy, providing a promising avenue for future research aimed at utilizing low-temperature thermal energy.

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PY-GreenChem-07

Sustainable synthesis of carbon materials doped with heteroatoms and non-precious metals from biomass residues for energy generation

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Introduction

Replacement of fossil fuels by renewable energy is mandatory to mitigate the climate change mainly originated by the emission of CO_2 to the atmosphere. Considering the intermittency of renewable energy, the development of efficient energy storage devices is necessary for their deployment. Among the energy storage and generation technologies, electrochemical devices are one of the most studied because of their versatility and efficiency. Among them, batteries, supercapacitors, electrolyzers and fuel cells are under continuous research and development to improve their capacity to store or produce energy without compromising the power or stability. In most of these devices, electrocatalysts are necessary due to the slow rate of the reactions involved and these catalysts are usually based on precious metals supported on carbon materials. This requires the use of high amounts of precious metals that impede the implementation of the technology. In this sense, new catalysts either based on metal-free carbon materials or non-precious metal-based catalysts are subject of strong research trying to find materials that can substitute precious metals and that use greener and more sustainable processes [1].

Nitrogen-doped carbon materials and non-precious metals have demonstrated their electrocatalytic efficiency and their capacity for application in multiple scientific, technical and industrial fields. These materials emerge as a promising alternative to platinum-based electrocatalysts used in the Oxygen Reduction Reaction (ORR) [1]. The presence of nitrogen increases the selectivity of carbon materials towards a 4-electron pathway, a thermodynamically-more-favoured and more desirable mechanism, and allows interaction with the incorporated metal, which in turn promotes the formation of new active sites [2,3]. In this study, catalysts were prepared with different amounts of carbon material (derived from a biomass residue), nitrogen precursor, and metal precursor, which in this case were dicyandiamide and iron oxalate, respectively. Ground almond shell (AS) was used as precursor of carbon materials and the results were compared with catalysts prepared with a high porosity activated carbon. For the synthesis, a mechanochemical treatment and a further thermal treatment at different temperatures were carried out, being this process easier and more environmentally friendly than the conventional solvothermal methods typically used.

Physicochemical and electrochemical characterization have shown that performing a mechanochemical treatment prior to the temperature program allows the incorporation of the precursors into the carbon material with better Fe distribution, and that humidity conditions and milling duration are key factors in the outcome of the samples. The materials prepared show interesting electrocatalytic properties, being a methodology that could be optimized for further scaling-up.

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PY-GreenChem-08

Exploring the potential of a deep eutectic solvent and a magnetic deep eutectic solvent for the determination of bisphenols in edible oil samples

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Introduction

Bisphenols (BPs) constitute a class of synthetic organic compounds that are primarily utilized as additives in the manufacture of epoxy resins, polymers, and a variety of food packaging materials. However, these compounds have the potential to leach from packaging into food, which could result in significant health risks due to their adverse effects on reproduction, metabolic development, the nervous and immune systems, and cardiovascular diseases [1]. Initially, the adverse effects of bisphenols were mainly attributed to bisphenol A (BPA), but it has been discovered that BPA analogues also possess similar toxic properties [2].

The aim of this research is to develop and validate two analytical methods based on vortex-assisted dispersive liquid-liquid microextraction (VA-DLLME), employing a deep eutectic solvent (DES) and a magnetic deep eutectic solvent (MDES) as extractants, followed by separation and detection via liquid chromatography with a diode array detector (LC-DAD). The use of VA-DLLME as an extraction technique offers several advantages, including high extraction efficiency, low solvent consumption, and simplicity. Additionally, the utilization of DES and MDES as extractants presents a number of advantages over traditional organic solvents due to their biodegradability and reduced toxicity, making them an attractive alternative for green analytical chemistry applications. Furthermore, the appeal of using MDES as an extractant lies in its unique combination of environmentally friendly properties of DES, along with the benefits of magnetic extractants, which facilitate easier handling and recovery using an external magnetic field. This approach simplifies the extraction process, reducing both time and energy consumption.

This study compares the extraction process, method validation, and analysis of real samples using a hydrophilic DES composed of choline chloride and ethylene glycol (ChCl:EG, 1:2) and a hydrophilic MDES composed of choline chloride, ethylene glycol, and iron (III) chloride ($ChCl:EG:FeCl_3$, 1:4:1). The aforementioned solvents were used to determine the presence of four bisphenols (BPA, BPF, BPAF, and BPAP) in edible oil samples, including olive, sunflower, soybean, rapeseed, and sesame oil.

Acknowledgements

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PY-GreenChem-09

Micro-flow synthesis of a formulation of phosphorus fertiliser to enhance p content in soil and p uptake in wheat

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Introduction

Highly soluble commercial phosphorus (P) fertilisers have been the most common form of P applied in agricultural for decades, but their releasing efficiency can be low because phosphate ions can be easily bound with cations in soil to form precipitates or highly water soluble species, leaching into nearby water sources causing eutrophication. Using the coiled flow inverter (CFI), a new formulation of phosphorus fertiliser was prepared containing three main components: a solid P source (biphasic calcium phosphate), a soil remediation agent (citrate ions) and a binding agent (chitosan). Our paper is one of the first fertiliser performance material made in flow that is a finished product comprising structural and functional complexity and we demonstrate its performance by soil experiments. We show proof of concept at scale to a complex product, which is amenable to open door to a commercial application. The key factors to evaluate the prepared fertiliser were P releasing efficiency, soil available P and P uptake. The prepared formulation tripled the available P in soil applied with commercial apatite (probability value, $p\text{-value} < 0.05$) and reached the same level with commercial P fertiliser in the incubation experiment. After incubating for 14 days, 63% of the applied P in the prepared fertiliser was released in the soil. The formulation without chitosan exhibited higher uptake of P in Scepter wheat in comparison with phosphate rock. In the soil column experiment, the commercial P fertiliser leaked double the amount of phosphorus after 23 days and had a fluctuated releasing behaviour when compared with the prepared formulation. Batch and flow synthesis (8 mL min^{-1}) share similar green chemistry metrics, including E-factor of 0.4 kg kg^{-1}. Continuous-flow production for CS-ACP-Cit has higher productivity than batch by a factor of 1.9. Circularity of the process, denoted by Materials Circularity Indicator (MCI), when considering experimental recycling data, is high for all process steps and all composites, scoring in the range of 0.8; also seeing this is a non-optimised process. The circularity assessment took account for performance of composites, which is expressed as Intensity Factor (U; performance) and Lifetime (L) of the Materials Circularity Indicator (MCI).

Acknowledgements

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PY-GreenChem-10

Functionalized cellulose from deproteinized soybean hulls as an environmental decontamination and disinfection tool

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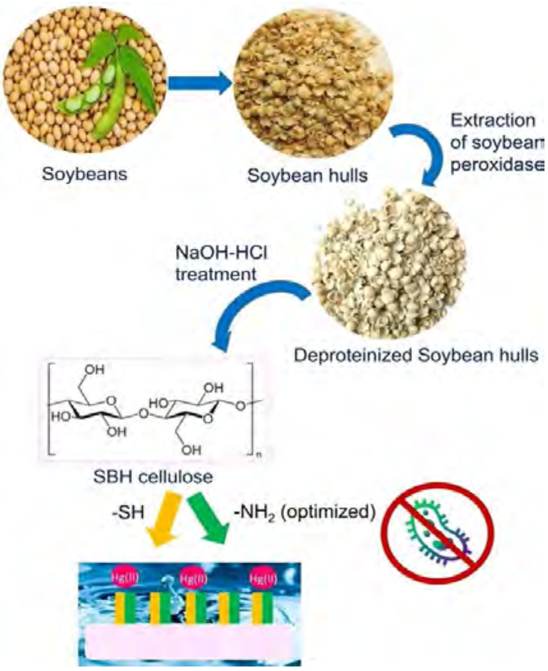
Introduction

Soybean hulls (SBHs) are one of the main by-products of soybean crushing, usually destined for animal feeding or to become a putrescible waste. In this work, we upgraded the waste SBHs to materials able to (i) act as antibacterial agents and (ii) adsorb mercury from wastewater, following the pathway represented in the scheme below.



In order to achieve these goals, the first step was the extraction and recovery of soybean peroxidase, since it is an enzyme naturally present in soybean hulls and finds application in different technological sectors [1,2]. Then, the exhausted lignocellulosic biomass was chemically treated to isolate cellulose powder, which was further processed by introducing amino (SBC-NH_2) and thiol groups (SBC-SH) through optimized procedures. Indeed, particularly in the case of amino-functionalized cellulose, it was found that the functionalization methodology in terms of solvent type, reaction temperature (strictly connected to the solvent characteristics) and amount of attached amino groups strongly influenced the final characteristics of the materials.

SBC-NH_2 powders were then successfully employed, even in low concentration, against gram-positive (Staphylococcus aureus) and gram-negative (Escherichia coli) bacteria, leading to the complete disinfection practically in all cases studied [3].

SBC-NH_2 was also tested, together with SBC-SH, as a Hg adsorbent in the water matrix. Both the samples showed a relevant adsorption capacity at pH between 5.5 and 8, but SBC-SH ensured a higher mercury removal also in an acidic environment. Preliminary tests in real water samples (effluent from the secondary treatment of a Wastewater Treatment Plant) are under investigation.

Acknowledgments

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P-SustDev-01

How design thinking applied to project co-creation with systems stakeholders enhanced the methodology for the CRAWL walkability project

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Introduction

University campuses built environments are reflective of the eras they were built. Like residential neighbourhoods since the 1960's, university campuses have become increasingly suburban and car dependent. The CRAWL (Campuses Role as Actors in Walkable and Liveable communities) project sets out to use TU Dublin's three main campus locations as a test bed for an action research living labs project with scalability not just to other educational campuses, but to other campus sites such as business and health. With the Office of the Planning Regulator as Societal Impact Champion, a design thinking process was undertaken with stakeholders from government, local authorities, advocacy and community across disciplines including engineering, planning, transport, health promotion and environmental monitoring.

The diverse and unique range of stakeholders hosted at each campus pose a unique set of opportunities and challenges for stakeholder engagement, with unique local knowledge and contexts between each campus, all of which are located within different administrative local authorities working in silos. The CRAWL project has resulting utilised this challenge as an opportunity of learning for understanding how to engage a broad scope of stakeholders to co-create design thinking approaches of achieving walkability and liveability in the campus setting. This poster presentation will outline approaches of how unique stakeholders were engaged with in each campus context, highlighting the common ground that emerged from engagement and issuing recommendations on how to communicate with stakeholders in future projects that aim to deliver on walkability through the co-creation of solutions.

Acknowledgements

This project is funded by Taighde Éireann - Research Ireland under the National Challenge Fund's Sustainable Communities Challenge. This project is supported by our Societal Impact Champion, the Office of the Planning Regulator.

P-SustDev-02

Geochemical characterisation of peloids and ecosystem services of peloids-rich areas in Serbia

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Introduction

Peloids represent "mature" mud, which consists of a complex mixture of fine-grained natural materials of geological and/or biological origin and mineral water. The quality of peloid and its potential application in pelotherapy depends on its thermal, chemical and mechanical properties, and the specifics arise from the composition and interaction of the inorganic and organic part with mineral water during the maturation processes, as well as from the conditions in the sedimentation environment. These processes are accompanied by biological activity, which additionally changes the composition of the organic and inorganic parts of the peloid. They can form in lakes, wetlands, seashores and floodplains, as a result of volcanic and hydrothermal activity. Peloids or healing muds are considered economically valuable natural resources that are used for therapeutic, cosmetic and relaxation purposes.

In Serbia, there are over 50 spas with over 1000 sources of different mineral waters, the differences of which result from different geological compositions and hydrogeological and geothermal characteristics. Some spas, in addition to healing waters, also have healing mud and gas, and some are air spas thanks to their geographical location. Although peloids have been used for therapeutic purposes in Serbia since ancient times, they have not been sufficiently investigated. There is no systematic and comprehensive peloid database with their physicochemical, geochemical and ecochemical characterisation.

The main goals of the project "Peloids in Serbia: geochemical characterisation, quality assessment and ecosystem services of peloid-rich areas (PELAS)" are to determine the geochemical and ecochemical characteristics of peloids from commercial spas in Serbia to determine: (i) the geological history and conditions of the sedimentation environment that contributed to their formation; (ii) the composition of the peloids and to assess their suitability for use, (iii) the assessment of the ecosystem services of areas rich in peloids, and (iv) to form systematic and comprehensive Data-point map. Within the PELAS project, healing mud from 15 spas covering all regions of Serbia will be analysed [1].

The expected results of the PELAS project are the characterisation of peloids, based on which it is possible to give guidelines for their use; reconstruction of the sedimentation environment and geological history that contributed to the formation of peloids, based on which it is possible to find new potential deposits of peloids; assessment of ecosystem services that will provide a basis for local stakeholders to understand the potential of peloid-rich areas that can contribute to their sustainable management and better exploitation following the sustainable use of natural resources, e.g. through ecotourism; The Data-point map will contain all information about the analysed peloids and the investigated area; it can have a medium and long-term impact on existing knowledge about peloids and be the basis for further research in the field of geochemistry, medicine, tourism, etc.

Acknowledgements

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P-SustDev-03

Characterisation of the liquid fractions obtained in the co-pyrolysis of waste from corn and polystyrene

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Introduction

It has become an attractive approach to mix biomass and plastic waste as feedstocks for the co-pyrolysis process, from the view of waste management and circular bioeconomy concepts. The demand for fuel sources is increasing, which has directed research towards this area [1]. The pyrolysis of waste biomass offers one potential solution for producing bio-oil, which can exhibit some fuel-like properties [2]. However, improving the resulting products' characteristics is necessary due to the high content of oxygenated compounds from biomass (lignin, cellulose, hemicellulose) [3]. To address this, an additional step is introduced to enhance the properties of bio-oil obtained from the pyrolysis of waste biomass by adding compounds such as plastic polymers from plastic waste, which contain only C and H, to increase the proportion of these elements in the final product [4].

This study examines the co-pyrolysis of corn from biomass waste with polystyrene from plastic waste, mixing in three different ratios of biomass to plastic (90:10; 70:30; 50:50). To follow the effect of co-pyrolysis yield, calorific value, some physical-chemical properties (pH, ash and moisture content) were also analysed. The presence of functional groups in the liquid fraction was characterised using FTIR analysis, while GC-MS analysis was used for compound identification. Adding polystyrene to corn waste biomass affected the increase in the liquid fraction yield, which was 32.60% with 10% added polystyrene. In comparison, the liquid fraction yield in the sample with 50% polystyrene was 47.88%. The heating value increased with the higher proportion of added polystyrene, from 23.58 MJ/kg with 10% polystyrene to 28.19 MJ/kg with 50% polystyrene, indicating that the heating value rises as the carbon and hydrogen content increases.

Compared to previous studies, progress has been made by adding polystyrene as a source of C and H to increase their proportion in the liquid fraction and obtain higher-quality bio-oil with oxygen-free compounds, revealing a synergistic effect. Based on the results, it can be concluded that improvements have been made compared to using biomass alone. However, further research should focus on adding catalysts to make the pyrolysis process even more efficient and extract valuable compounds from the raw material.

Acknowledgements

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P-SustDev-04

Assessment of ecosystem services potential of Serbian spas and peloid reach areas

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Introduction

Although people have always understood the value of nature, the term "ecosystem services" was established recently to encompass these many advantages. Any beneficial resource that ecosystems or wildlife offer humans is considered an ecosystem service. The advantages may be minor or major, direct or indirect. According to Millennium Ecosystem Assessment (MA), there are four major categories of ecosystem services: provisioning, regulating, cultural and supporting services.

Frequently, decision-makers fail to recognize the importance of ecosystem services. We can ensure that decision-makers acknowledge the benefits of natural ecosystems by implementing a systematic approach that includes evaluating ecosystem services. Employing the assessment of ecosystem services, it is possible to raise awareness regarding the imperative of nature conservation [1].

The main goal of this study is to find the answers to the following questions: Which non-economic, economic, and potential benefits can be provided by spas and peloid reach areas in Serbia? The study was developed in the entire territory of the Republic of Serbia, covering four areas and 15 spas: North (Kanjiža, Rusanda, Junaković), Central West (Koviljača, Vrujci, Selters, Ždrelo), South West (Lukovska, Kuršumlijska, Prolom, Jošanička), and South (Niška, Sijarinska, Vranjska, Bujanovačka). In evaluating the full range of current and potential values of these areas, the PA-BAT+ methodology was performed by collecting the data through questionnaires for various stakeholders [2].

Results showed that ecosystem services in different studied areas are recognised to come from different groups of services depending on the geographical position, type of terrain, proximity to cultural and historical monuments, known tourist attractions, and geopolitical position. The evaluation, conducted using the PA-BAT+ approach, provides a reasonable foundation for obtaining all essential information on the characteristics and operation of spa areas. The gathered information might also help identify the major problems and obstacles to the integrated management of spas. The results of this study can be used at both local and national levels to improve governance and to progress appropriate policies that support nature conservation while promoting sustainable development and responsible use of natural resources. They also serve to promote effective communication and cooperation among various parties. The results of this study could be used to raise awareness of the significance of spa areas for the tourism and economic development of the entire country.

Acknowledgments

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P-SustDev-05

Amine cross-linked *Opuntia* biomass for enhanced nitrate adsorption performance

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Introduction

Water is essential for life. The importance of water as a resource for life and sustainable development is well established. Around the world, agriculture is the leading cause of water degradation. Nitrate pollution, mainly due to excessive use of nitrogen fertilization, leads to the degradation of both surface and groundwater, making it one of the most concerning environmental problems at present around the world, attracting considerable research interest [1,2]. This is a particularly pressing problem in aquifers in the Region of Murcia, and particularly in the Mar Menor coastal lagoon (SE Spain). The adsorption process has been widely considered for pollutant removal in waterbodies because of its technical feasibility, simple operation, affordable costs, and the possibility of using multiple adsorbents of the most diverse nature [3]. Agrowaste by-products, as lignocellulosic biomass-rich materials, have stimulated new gateways for the production of renewable, low-cost and sustainable sorbents for water treatment applications. Although conventional agrowaste biomass generally do not have high sorption capacity, chemical surface modification can significantly improve the removal efficiency. To improve the adsorption capacity of the biomass against anionic species, surface treatment with amine groups is considered to be quite effective as it enhances the electrostatic sorbent-adsorbate interaction. The activation of the crude biomass was performed with epichlorohydrin, N,N-dimethylformamide, diethylene-triamine and triethylamine using the method of Wu and coworkers [4]. The effect of the functionalization on the sorbent capacity was studied in batch experiments. The objective of this work is to study the best conditions for nitrate adsorption in water using amine modified biomass from *Opuntia* cladodes.

The raw biomass was obtained from a local orchard, and after drying, grinding and sieving, different particle size fractions were selected. A three-factor three-level Taguchi analysis design (Table 1) was used to establish the optimum conditions of the sorption process.

Table 1. Factorial design matrix

Factor	Level 1	Level 2	Level 3
A. Sorbent dosage (g/L)	0.5	1.0	2.0
B. Initial nitrate concentration (mg/L)	50	200	400
C. Particle size (mm)	0.25-0.50	0.50-0.85	0.85-1.00

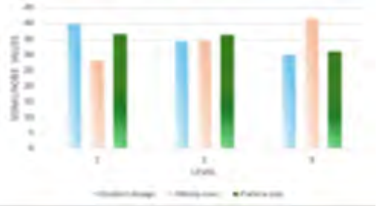

Fig. 1.- S/N ratios for adsorption capacity (q_e)

The amine-modified biomass was characterized by field emission scanning electron microscopy (FESEM) and Fourier transform infrared spectroscopy (FTIR). The result of the Taguchi DOE approach (Fig. 1) revealed the optimal operative conditions to obtain the highest sorption capacity. The amine-functionalization process was effective as shown by the differences in the infrared spectra before and after modification. The enhancement achieved in the nitrate adsorption capacity, with respect to that shown by the raw *Opuntia* biomass, is to be highlighted, going from 10 to 142 mg of nitrate ions per gram of sorbent biomass, which corresponds to an increase of more than 1400%.

Acknowledgements

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P-SustDev-06

Physicochemical characterization of insulating plastics: a step towards a circular approach to cable recycling

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Introduction

Metals from waste cables are separated from insulation plastic by open burning in many locations in Serbia. Such practice is the cause of air pollution by a series of carcinogenic substances and particulate matter (PM10, PM2.5, and PM1.0) unequivocally linked to the high incidence of diseases and greenhouse gas emissions. Several recycling companies have only recently started mechanically separating metals and insulating plastics. However, this is only the first step in achieving circularity and maximum utilization of waste cables. A circular approach will be established only when the insulating plastic, which still has no use value, finds reuse. Determining the composition of waste cables is a critical step in the recycling process. In this work, cables were manually separated and sorted by external appearance and color into clean streams (Figure 1). The copper was mechanically separated from the plastic. The shredded plastic was analyzed using infrared spectroscopy (IR) to determine the type of polymer. Eight of 11 waste cable samples were based on polyvinyl chloride (PVC), while three were based on polyethylene (PE). The thermal properties of the sorted polymers, such as the glass transition temperature (Tg) and the melting temperature (Tm), were investigated using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). These analyses provided insight into the thermal stability, which is necessary to process specific waste polymers. The thermoplastic part of the plastic can be regranulated and reused to produce items such as flower pots and trash cans. In contrast, cross-linked plastic could be used in asphalt production, enabling the full utilization of insulating plastic.

Figure 1. Insulated plastic sorted into clean streams

The outcome of this work provides a detailed understanding of the composition, structure, and properties of the insulating plastic after the copper has been removed, as well as the identification of the types of polymers that enter the composition of the plastic. Based on this, concrete recommendations can be made for the reuse of insulating plastic. The main goal is to highlight the potential for the reuse of this plastic, which would motivate recycling companies to separate insulating plastic by polymer type and deliver it to regranulate manufacturers. These results help establish a circular approach to cable recycling, which would prevent significant pollution caused by their burning at numerous locations in Serbia.

Acknowledgements

This work is supported by the UNDP grants: “EcoCableRecycling: Sustainable and efficient management of cable insulation plastic”, No: 001363377/00127312/2023/21 and Circular Vaucher for 2023: “Physico-chemical characterization of insulating plastic and possibilities of its use - circular approach to cable recycling”.

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P-SustDev-07

Investigating the formation of silver nanoparticles by freshwater microalgae

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Introduction

The release of engineered silver nanoparticles (AgNPs) into aquatic environments has increased in recent years due to their accelerated production and incorporation into commercial products, such as clothing, electronics, sports equipment, and for their important medical applications [1]. AgNPs tend to dissolve, leading to the coexistence of particulate and dissolved silver in aquatic environments. Although their potential detrimental effects on aquatic organisms have been widely studied, information on the influence of phytoplankton on the cycling of AgNPs is limited. In addition, microalgae have been shown to act as "green factories" of metallic nanoparticles from dissolved metals, including Ag^+ [2,3]; however, the mechanisms involved in their formation are not yet fully understood.

This research investigates the *de novo* formation of AgNPs by the freshwater phytoplankton species *Cyclotella meneghiniana* (diatom), *Chlamydomonas reinhardtii* (green alga), and *Rhaphidocelis subcapitata* (green alga) from ionic silver Ag^+, focusing on both extra- and intracellular synthesis. The size, dissolution, and aggregation trend of the newly-formed AgNPs were determined using Scanning Electron Microscopy (SEM), Dynamic Light Scattering (DLS) nanoparticle analysis, Asymmetric Flow Field Flow Fractionation (AF4) and Surface Plasmon Resonance (SPR).

The results demonstrated that algal secretions play a crucial role in the synthesis of AgNPs from Ag^+. Incubation of *C. reinhardtii* and *C. meneghiniana* exudate solutions with various concentrations of $AgNO_3$ (ranging from 50 to 200 ppm) clearly resulted in the formation of AgNPs. Nanoparticles were detected after 6 to 24 hours of incubation, depending on the species producing the exudate, and remained stable for more than a week. The characteristics of the *de novo* synthetized AgNPs were specific to the composition of the exudates, varying from one species to another. In the other hand, incubation of *R. subcapitata* exudate solution with $AgNO_3$ resulted in weak production of AgNPs, which exhibited low stability over time. The protein content in the exudate appears to play a key role in AgNPs synthesis: higher protein concentrations in the exudate solution correlate with stronger detection of newly-formed nanoparticles.

AgNP formation was not detected when exudate-free microalgal suspensions were incubated with $AgNO_3$. It is possible that nanoparticles were present but in concentrations too low to be detected with the techniques used so far (AF_4 and SPR). To further investigate the cellular-mediated AgNP formation, including their potential intracellular formation, we tracked the time course of Ag^+ adsorption and internalization by *C. reinhardtii* and *C. meneghiniana* after optimization of the cell washing procedure. Results show a rapid uptake of this metal, reaching the plateau after two hours in both species. The intracellular Ag concentration of *C. meneghiniana* was four times higher than for *C. reinhardtii* (5×10^{-17} vs 2×10^{-16} mol/cell). Finally, experiments where cytosol extracts of *C. reinhardtii* were incubated with Ag^+ resulted in the formation of AgNPs, indicating that nanoparticle formation could also happen intracellularly in this species.

Acknowledgements

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PY-SustDev-01

A simple and eco-sustainable synthesis approach for the development of electrodes for highly durable supercapacitors

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Introduction

The wide spectrum of multifunctional materials that can be synthesized from carbon has led to the success achieved in recent decades in the development of new highly durable materials for use as electrodes in supercapacitors. However, despite significant advances, in most cases the preparation of these materials usually requires complicated or lengthy synthesis routes, which go hand in hand with high-tech and high-cost equipment as well as the use of environmentally unfriendly chemicals. To comprehensively evaluate the environmental impacts generated by the process and identify opportunities for additional improvement, this research focuses on applying the Life Cycle Assessment (LCA) methodology to the synthesis process to produce dual nitrogen and phosphorus co-doped activated carbons[1]. The synthesis of these materials is carried out by conventional chemical activation with H_3PO_4 using chitosan as precursor, given that it is one of the most abundant carbon sources in nature and has a significant nitrogen content in its structure.

It is important to highlight that the preparation process used not only reduces the environmental impact, but also allows the co-doping of the carbon network, improving the electrochemical performance of the resulting activated carbon when used as electrodes in supercapacitors. The most powerful advantage of this approach is its high efficiency as it involves few synthesis steps compared to other reported studies.[2–4] Such a simple methodology results in N,P-doped activated carbons with high yield and excellent textural properties (S_{BET} =1515 m^2 g^{-1}), and nitrogen and phosphorus contents of 2.3-3.3 at% and 0.4-0.6 at%, respectively, being used to prepare electrodes as supercapacitors in an organic electrolyte. The assembled symmetric supercapacitor exhibits outstanding electrochemical stability due to the dual effect of both heteroatoms, showing that these devices have excellent durability after 10000 charge-discharge cycles with energy and power comparable to a commercial activated carbon (YP50F) used for this application. In this sense, these carbon materials obtained from biomass could be considered as a sustainable alternative to develop efficient energy storage devices that would compete with those materials used in commercial supercapacitors.

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PY-SustDev-02

Elemental analysis of environmental samples by means microwave-sustained inductively coupled atmospheric-pressure plasma optical emission spectrometry

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Introduction

Microwave-induced plasma optical emission spectrometry (MIP-OES) has become increasingly popular for trace element analysis as a cost-effective alternative to inductively coupled plasma optical emission spectrometry (ICP-OES), largely due to its use of nitrogen as the plasma gas. The employment of nitrogen contributes to a more sustainable practice by reducing dependence on rare gases like argon, promoting a greener approach to plasma-based elemental analysis. Among the latest developments in MIP technology is the microwave-sustained inductively coupled atmospheric-pressure plasma (MICAP), which maintains an annular plasma similar to ICPs via a dielectric resonator ring and a 2.45 GHz microwave field. While MICAP-OES has demonstrated detection capabilities on par with ICP-OES, its application for real-world environmental samples with complex matrices, including mining-related samples, remains underexplored.

This study evaluates the performance of MICAP-OES for the elemental analysis of various environmental samples, emphasizing the robustness of the technique in the presence of challenging matrices such as organic/inorganic acids and saline matrices. Nineteen elements (Ag, Al, As, B, Ca, Cd, Co, Cr, Cu, Fe, Ga, In, Mg, Mn, Ni, Pb, Sr, Tl, Zn) were analyzed in simulated matrices (sulfuric acid, hydrochloric acid, acetic acid, sodium chloride, calcium chloride), commonly encountered in sample preparation or naturally present in environmental samples.

Plasma experimental conditions and calibration strategies were optimized in order to mitigate both spectral and non-spectral interferences, and various certified reference materials were analyzed, including BCR-146 (industrial sewage sludge), BCR-483 (sewage sludge-amended soil), BCR-278R (mussel tissue), CRM-DW1 (drinking water) and OREAS 112, 282 and GBM310-2 (metallic ores).

MICAP-OES exhibited lower susceptibility to signal variations caused by easily ionizable elements in saline matrices compared to other MIP systems. Moreover, it was observed that the optimum nebulizer gas flow rate for both atomic and ionic wavelengths was mostly independent of matrix characteristics. The simultaneous spectrometer configuration also allowed for efficient internal standardization, further enhancing the technique's capability to deliver accurate and reproducible results. Finally, results showed that MICAP-OES is highly resilient to matrix effects, with recovery rates between 90% and 110% across all tested CRMs, demonstrating its suitability for complex environmental and mining sample analysis.

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PY-SustDev-03

HOW to renew, WHAT to transform, WHOM to help – KAJ KO BI

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Introduction

The Interdisciplinary Student Projects for Sustainable Development, titled "HOW to Renew, WHAT to Transform, WHOM to Help Live" (abbreviated as KAJ KO BI), brought together in workshop activities three groups—young adults (students), active adults (professors), and older adult participants with a common aim to bridge the generation gap for a sustainable future. The workshops were designed to explore various ways in which a circular economy, as opposed to a linear one, can enhance the social inclusion of vulnerable groups and promote the sustainable use of resources.

Students and professors represented the young and active participants from different study programs: occupational therapy, sanitary engineering, and textile design, whereas the vulnerable group of older adults came from a Home for the Older Adults Fužine, located in Ljubljana. This collaboration allowed future therapists, engineers, and designers to test themselves in a real environment and co-create a space of health, creativity, self-expression, inclusion and well-being through various interdisciplinary activities. The creative workshops were based on the reuse of surplus textile materials, which, along with waste electrical and electronic equipment, are among the fastest-growing types of waste in the European Union.

The 12 workshops were organized into 4 thematic areas, where students from each study programme developed their leadership skills by coordinating sub-activities that included participants of various ages and skill levels:

1. Introduction workshops highlighted the innovations of a technology-driven society by employing analytical methods to determine the polymer composition of various materials. Textiles were characterized, then separately processed and transformed into new items that can be made by both young and older adults, including those with health or age-related vulnerabilities.
2. HOW to Renew workshops were focused on natural dyes found in nature and the creation of new products from natural materials or refreshed old textiles emphasizing alternatives to the wastefulness of fast fashion.
3. WHAT to Transform workshops involved activities of transforming fossil-based plastics into new, useful household items.
4. WHOM to Help Live workshops included activities to maintain motor, process, and social interaction skills through simple products made from natural and synthetic materials. These workshops were based on the socializing skills of all participants and the beneficial impact of intergenerational exchange of experiences, contributing to the mental health of both young and older adult participants, and allowing them to share their own experiences and skills. This process fostered creativity, connection and emotional well-being and contributed to the mental health of all groups.

The rotational structure of the workshops allowed all students to use technically demanding equipment provided direct experience working with the older adults, and introduced creative techniques available in the artistic environment. The project was part of a broader approach to social sustainability, inclusion, and the circular economy, aligning with the goals of the 2030 Agenda for Sustainable Development [1,2].

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PY-SustDev-04

Assessment of a deep eutectic solvent for liquid-liquid microextraction of six pharmaceuticals form wastewater

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Introduction

In recent decades, the ubiquitous presence of pharmaceutical products (PPs) in aquatic environments, including seawater, wastewater, and groundwater, has emerged as a significant environmental concern. These contaminants, such as antibiotics and non-steroidal anti-inflammatory drugs (NSAIDs), pose significant risks to human health and aquatic ecosystems while challenging conventional water treatment technologies [1]. Commonly detected pharmaceuticals, including ampicillin (AMP), ciprofloxacin (CIP), sulfamethoxazole (SMX), diclofenac (DIC), naproxen (NAP), and ibuprofen (IBU), require an exhaustive sample preparation to extract them from complex matrices [2].

To address the drawbacks of traditional solvents, this study presents a novel and environmentally friendly approach using thymol (THY), a natural phenol, combined with water to form a deep eutectic solvent (DES), which was characterized by ATR-FTIR, TGA and NMR to confirm the formation of DES [3].

This DES-based method offers improved extraction and detection efficiency while promoting sustainable analytical practices. In addition, the proposed method was evaluated using the AGREE prep tool, which evaluates methodologies based on the ten principles of green chemistry, contributing to a more sustainable and environmentally friendly approach in analytical chemistry [4].

The extracted compounds were further analyzed using UHPLC-DAD. The DES-based method demonstrated better performance compared to traditional solvents, highlighting its potential for sustainable applications. This study presents a novel approach to liquid-liquid microextraction (LLME) using hydrophobic DES for the efficient extraction of various PPs, including antibiotics and NSAIDs, from wastewater using a sample volume of 10 mL and a DES volume of 200 µL. The DES composition was optimized to achieve optimal extraction conditions, including sample and elution volumes, resulting in a preconcentration factor of up to 20. The method was validated by rigorous evaluation, presenting low method detection and quantification limits (DIC 1.03 and 3.45, SMX 1.09 and 3.66, IBU 2.07 and 6.91, AMP 2.36 and 7.86, NAP 3.26 and 10.87 and CIP 9.78 and 32.60 µg L^{-1}), a wide linearity range (35 to 2000 µg L^{-1}), good precision inter and intraday (≤ 4.1 % RSD), $R^2 > 0.993$ and recoveries between 75 and 96%. The AGREE Prep score was also calculated, yielding a result of 0.60.

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