EMEC17
Inverness 2016

17TH EUROPEAN MEETING ON ENVIRONMENTAL CHEMISTRY

November 30th – December 2nd 2016 • Inverness, Scotland

Book of Abstracts

Organised By

eri environmental research institute

University of the Highlands and Islands
Oilthigh na Gàidhealtachd agus nan Eilean

North Highland College
University of the Highlands and Islands

On Behalf Of

ASSOCIATION of CHEMISTRY and the ENVIRONMENT


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Welcome

Dear Colleagues

On behalf of the Organising Committee it gives me great pleasure to welcome you to Inverness, Scotland and to the 17th European Meeting on Environmental Chemistry in Inverness, Scotland. This will be the second time that the ‘capital of the Highlands’ has hosted and EMEC conference and we extend an equally warm welcome to both returning colleagues and to delegates visiting for the first time.

EMEC 17 will provide a forum for the exchanges of ideas on recent advances in research and development in environmental chemistry and technology, for people from academia, research, and industry. With invited key-note lectures, podium and poster presentations, the scientific programme of the conference will provide delegates new insights into some contemporary issues in environmental chemistry.

The scientific programme for EMEC17 will be based at Eden Court Theatre on the banks of the River Ness in the city centre. Here we aim to stimulate lively discussion and promote networking with colleagues from across Europe. We hope that the event will also instigate new collaborations as well as providing the opportunity to renew contacts with old friends from the EMEC community.

As well as the scientific programme a full social programme has been organised to allow delegates to experience some of the culture, food, and drink of the Highlands and Islands of Scotland. This will commence with the opening ceremony and welcome reception on the opening day of the conference. On the second day you will already have chosen whether to join a tour to Urquhart Castle overlooking the famous dark waters of Loch Ness; or to visit Glen Ord Distillery and sample some rather special ‘uisge-beatha’, the ‘water of life’. We conclude our conference in the Pavillion at Strathpeffer with a special dinner and cèilidh.

We very much hope that you will find the combination of scientific programme and social events proves to be rewarding and enjoyable from both professional and personal perspectives.

With best wishes

Stuart W. Gibb

Prof. Stuart Gibb
Chair of Organising and Scientific Committees
EMEC17

The 17th European Meeting on Environmental Chemistry

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ASSOCIATION OF CHEMISTRY AND THE ENVIRONMENT

The European Association of Chemistry and the Environment (ACE) is an European non-profitmaking scientific association founded in October 2000 by a group of European scientists. Aiming at the protection of the Environment, it will favour contacts between academics, education, private firms, and social representatives, working in the fields of chemistry, toxicology, agronomy, water science, sociology, etc....

... ACE wishes to promote in a balanced way the collaboration of scientists from all scientific fields aiming at the protection of the environment. Therefore we strongly welcome scientists from diverse fields such as biology, geology, sociology, toxicology, soil science, chemistry, water science, atmosphere science, geochemistry, medicine, etc.

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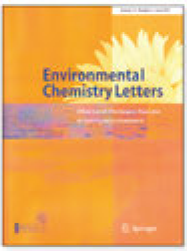
ACE MILESTONES

2000	October: ACE foundation.
2000	December: 1st European Meeting on Environmental Chemistry (EMEC1), Nancy, France - 1st Poster Award.
2002:	ACE Collaboration Network established among ACE members.
2003:	International peer-reviewed journal "Environmental Chemistry Letters" established (Springer Publisher); (2015 Impact Factor 2.573)
2004	November: Environmental Chemistry - A Springer book of articles from ACE Meeting.
2006	December: 7th European Meeting on Environmental Chemistry (EMEC7), Brno, Czech Republic - 1st Oral Presentation Award
2007:	Refoundation of ACE in Luxembourg
2010	December: 11th European Meeting on Environmental Chemistry (EMEC11), Portorož, Slovenia - 1st Pre –Conference Summer school.
2015:	**16th European Meeting on Environmental Chemistry (EMEC16), Torino, Italy; 1st ACE financial support for young perspective scientists**

PUBLICATIONS

Environmental Chemistry Letters is the official journal of the European Association of Chemistry and the Environment. This journal publishes short research and review articles.



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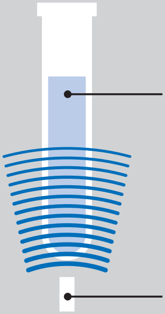

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General Information

ACCOMPANYING PERSONS

The accompanying person fee includes

- Welcome reception at Eden Court Theatre on 30 November
- Opening ceremony at Eden Court Theatre on 30 November
- Either of our two tours which will depart from Eden Court Theatre
- Conference dinner and ceilidh at the Strathpeffer Pavilion on 2 December
- Closing Ceremony and refreshments at Eden Court on 2 December
- VAT @ 17.5%

BADGES

The name badge issued to delegates on registration serves as an admission pass to all scientific sessions, the exhibition and inclusive social events. Delegates are asked to ensure that they wear their name badges at all times.

BUSINESS CENTRE

There is no business centre within Eden Court, should you require photocopying, faxing courier and freight solutions then please go to the EMEC17 registration desk.

CAR PARKING

Delegates will be able to utilise the Eden Court car park. This car park is barrier operated and will be complimentary to delegates during the conference, however this will be subject to availability of spaces.

CASH MACHINES

There are no cashs machines within Eden Court; the nearest cash machine is The Royal Bank of Scotland Plc which is located on Tormnahurich Street.

CERTIFICATE OF ATTENDANCE

A Certificate of Attendance will be available at the meeting. Please inform the EMEC17 registration desk if you require such a certificate

CLOAKROOM FACILITIES

There are cloakroom facilities next to the main ticket office within Eden Court; This service is complimentary to delegates throughout the conference.

CREDIT CARDS

Commonly accepted credit cards in hotels, restaurants and stores are American Express, Visa, MasterCard, and Diner.

DISCLAIMER

All best endeavours will be made to present the programme as printed. However, EMEC17 and its agents reserve the right to alter or cancel, without prior notice, any arrangements, timetables, plans or other items relating directly or indirectly to the conference for any cause beyond its reasonable control. EMEC17 and its agents are not liable for any loss or inconvienience caused as a result of such cancellation. Delegates are advised to take out their own travel insurance and to extend their policy to cover personal possessions as the conference does not cover individuals against cancellation of bookings or theft or damage to belongings. Tours run by third parties may be subject to cancellation should minimum numbers not be achieved.

ELECTRICITY

The voltage in the United Kingdom is 220-240v.

FIRST AID

There are dedicated first aid trained staff within Eden Court to assist delegates if required. In the event of an emergency please contact either a member of Eden Court staff or Concorde Services staff.

INTERNET FACILITIES

There is WiFi access throughout Eden Court which will be available to delegates on a complimentary basis.

INFORMATION DESKS

The main ticket office within the foyer of Eden Court also acts as an information desk should delegates require any assistance.

LANGUAGE

The official language of the conference will be English. No simultaneous translation will be available.

LOST PROPERTY

Enquiries regarding items lost or found can be made at the Registration Desk which is situated in the Bishops Palace. To minimise losses, please ensure that your Delegate Bag is labelled and that your name is written inside your copy of the Book of Abstracts

LUNCHES AND REFRESHMENTS

Coffee/tea and lunch will be served in the ‘stalls’ area near the One Touch Theatre This will also be where posters are on display..

MOBILE TELEPHONES

It should be noted that mobile phones must be switched off during scientific sessions.

PUBLIC TELEPHONES

There are no public telephones within Eden Court.

SCIENTIFIC SESSIONS

The Scientific Sessions will be held within the One Touch Theatre.

SMOKING POLICY

Smoking is not permitted within Eden Court. Should you wish to smoke then please do so outside the venue in the designated areas.

TAXIS

The telephone number for the local recommended taxi company, Highland Taxis is 01463 222 222.

VALUE ADDED TAX (VAT)

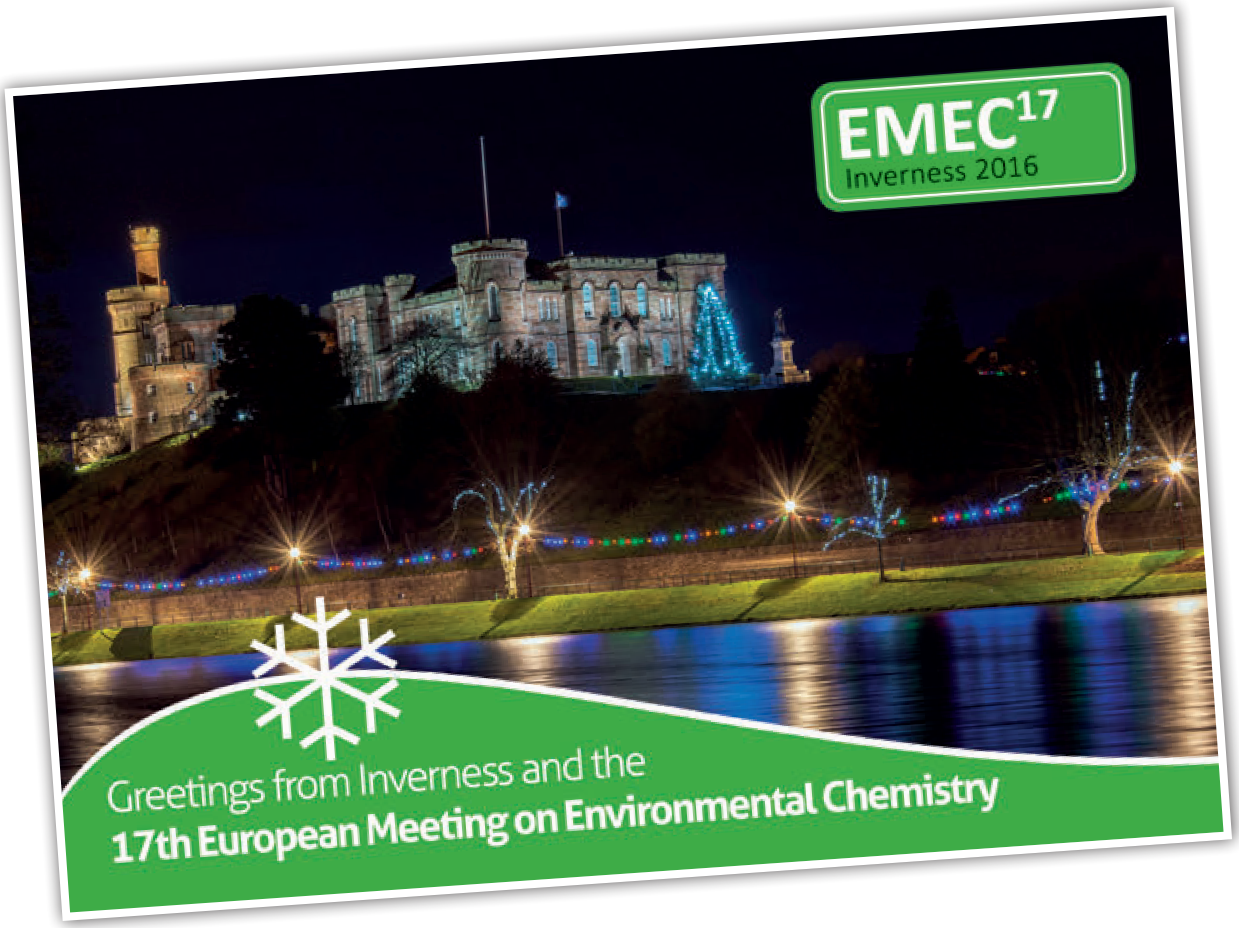
Value Added Tax and Similar taxes are charged on most goods and services in the United Kingdom. At the time of going to press, VAT in the United Kingdom is 20%.

Business travellers within Europe, subject to certain conditions, may reclaim VAT for Conference registration fees, accompanying persons’ registration fees etc. This applies to both non-European business travellers visiting Europe and to European business travellers to other EU countries. For further information please contact Customs and Excise on departure at the airport.

Social and Tours Programme

A detailed guide of the entire Programme along with information of the Tours are included in your welcome bag along with some fantastic items courtesy of our sponsors and ourselves.

Please make sure you let your colleagues and loved ones know what a wonderful time you are having at EMEC17 by sending them a postcard which we have provided in your welcome bag. (Stamps available at the EMEC17 Reception Desk)



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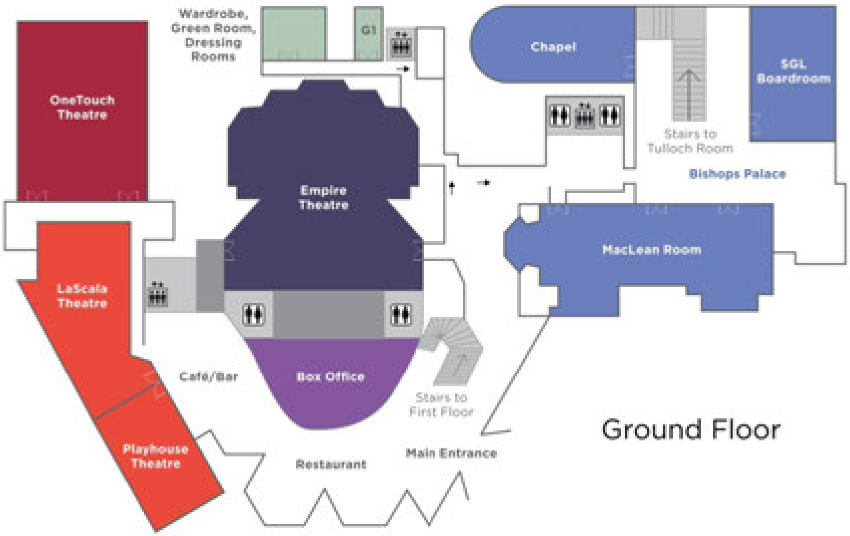

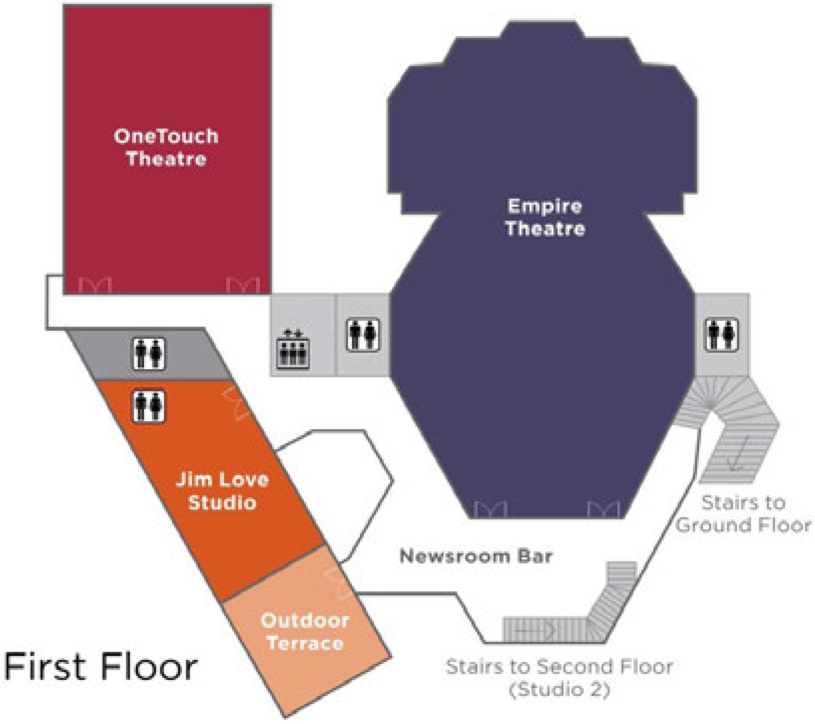

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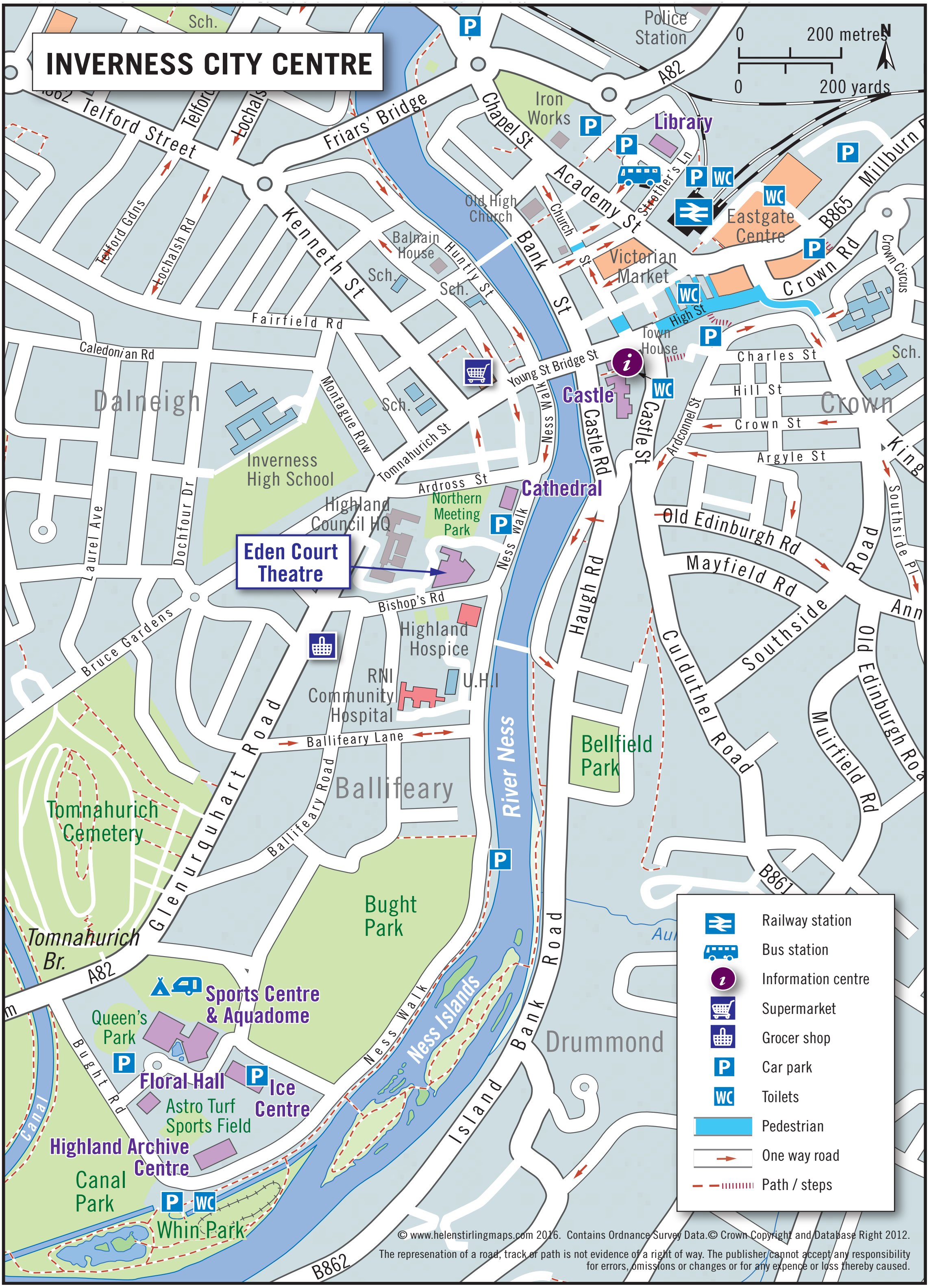

Keynote Speakers

Professor Phillip Whitfield

Professor Phillip Whitfield is Head of Lipidomics Research at the University of the Highlands and Islands in Inverness. He obtained his BSc in Biochemistry and Physiology from the University of Sheffield before going on to study for a PhD at University College London. His research has focused on the use of mass spectrometry to problems of fundamental biological and biomedical relevance. Key areas of his work include the development of LC-MS based global and targeted methodologies to study lipid metabolism in cell systems and complex organisms.

The title of Phillip's lecture is, "A Matter of Fat: The Development and Application of Lipidomic Workflows" in which he will examine the potential of lipodomics to provide new insights in environmental chemistry.

Professor Mike Billett

Advances in Environmental Chemistry - Opening the Black Box of Peatland Carbon Cycling

Mike Billett was appointed Chair of Biogeochemistry and Environmental Change at the University of Stirling in 2013 after 10 years at the Centre for Ecology & Hydrology (CEH), where he led the Carbon Catchments research initiative. Prior to joining CEH Mike was a Lecturer/Senior Lecturer at the University of Aberdeen. He has 30+ years of postdoctoral research experience with over 100 peer reviewed publications. His main research interest is in soil and surface water biogeochemistry, in particular the impact of soil processes, catchment management and environmental change on water quality. Recent research has focused strongly on northern hemisphere carbon cycling (particularly the Arctic and Scottish peatlands) at scales ranging from the water-atmosphere interface to catchment and larger scale regional studies of carbon transport. Approaches include field-based studies, application of isotopic methods, laboratory simulation and predictive modelling. Apart from the UK, he has carried out research in Fennoscandinavia, Canada, Greece, Ghana, Malaysia and Sri Lanka.

In his talk Mike will explore how significant advances in recent years (especially in radiocarbon dating of different carbon species) has led to a major change in our understanding of how carbon is stored, processed and released from organic-rich soils.

Professor Jörg Feldmann

Professor Jörg Feldmann has studied in South Africa (Jo'burg) on Geochemistry of gold, volatilisation of metals from landfill sites in Germany (Essen) and in Canada (Vancouver) on arsenic processes in the environment before coming to Scotland in 1997. Since then he is at the University of Aberdeen, Director of TESLA (Trace Element Speciation Laboratory) in the Chemistry Department and Professor for Environmental Analytical Chemistry. His main focus is the understanding of processes in the environment and in biological system in which arsenic, selenium and mercury and other metals are involved by developing novel analytical systems for which he has recently received the European Award for Plasma Spectrochemistry 2015 and the RSC Interdisciplinary Prize 2016. He has published more than 250 papers in more than 70 journals and receives annually more than 1000 citations.

Jörg will be presenting a talk entitled, "Should We Bother About Elemental Speciation in Environmental Studies?" The lecture will define elemental speciation and will explain the different approaches to determine the molecular structure of metals and metalloids in different environments.

Oral Presentations

OP 1

Peculiar Pollutants in the Moscow Atmosphere in Winter Period: a GC-HRMS Study

Albert Lebedev; D.M.Mazur; O.V.Polyakova; V.B.Artaev

Control of air pollution, especially in highly populated areas, is a vital task for the environmental authorities. Among the widely used methods of environmental analysis, mass spectrometry provides the best analytical results combining selectivity, sensitivity, reliability, and information capacity. The most common mass spectrometry approach dealing with environmental pollution involves targeted analysis, i.e. detection and quantification of preselected (priority) pollutants. However the non-targeted analysis has becoming more often the method of choice for the analysts. It involves implementation of the modern analytical instrumentation allowing identification of all compounds of environmental interest present in the sample at very low levels, such as pharmaceuticals and their metabolites, musks, nanomaterials, perfluorinated compounds, hormones, disinfection by-products, flame retardants, personal care products, and many other emerging contaminants. The present paper describes the detection and identification of previously never reported peculiar organic compounds in the snow samples collected in Moscow in March of 2016. Analysis of snow samples allows evaluation of the long term air pollution in the winter period.

Three snow samples were collected in March of 2016 near Lomonosov Moscow State University campus, Moscow, Russia. First sample represented a full depth snow layer collected near a busy highway, the second one was collected in the nearby park, and the third one was a sample of fresh snow, collected in the park. The first two samples were collected by piercing through the snow cover with a 10 cm internal diameter tube. The thickness of snow layer during the sampling was 30-35 cm. Sample 3 was collected during the snowfall by taking 5 cm deep of the upper layer of the fresh snow from the area of approximately 3 m^2.

All experiments were performed using time-of-flight high resolution mass-spectrometer Pegasus GC-HRT (LECO, USA). The system was controlled by the ChromaTOF-HRT® software version 1.91 (LECO Corporation), which was also used for spectra collection and data processing. The data were collected using 10 full (10-800 m/z range) spectra per second in high resolution mode (50000 at FWHH of m/z 219 peak), with high mass accuracy.

Notes

OP 2

Trophic Status of Greek Coastal Marine Environments (East Mediterranean) Coupled with Nutrient Stoichiometry and Human Pressures

Alexandra Pavlidou; Kalliopi Pagou; Eleni Rousselaki; Nomiki Simboura; Georgia Assimakopoulou; Manolis Tsapakis; Paraskevi Drakopoulou; Ioanna Varkitzi; Panayiotis Panagiotidis

Marine ecosystems are stressed not only by increased nutrient loads (eutrophication) but also by changing forms and proportions of nutrients. Indeed, anthropogenic pressures affected the coastal marine environments have significantly altered the nutrient loads and their composition. Changes in nutrient form and their stoichiometry both affect marine ecosystems' functioning resulting to undesirable effects (Glibert 2012 and references therein). In this work we have used data from 28 Greek coastal areas for the period 2012-2015, in order to assess the trophic status of the selected marine environments, affected by different human pressures, in relation to the nutrient stoichiometry and forms.

In general, ~48% of the study Greek coastal areas have been classified in Good trophic status, according to the chl-a classification system (Simboura et al. 2005), whereas ~30% of the study stations have been classified in Poor status, 9% at the High and Moderate status and only 4% in Bad status. Relatively lower DIN:P ratios (DIN stands dissolved inorganic nitrogen: nitrate + nitrite + ammonium) were recorded in the Greek coastal areas where some of the direct and indirect effects of eutrophication have been recognized (Pavlidou et al. 2015). For example, in Amvrakikos gulf hypoxic and anoxic conditions occurred, while in Thessaloniki bay (Thermaikos gulf) increased abundance of certain harmful dinoflagellate species was recorded.

The majority of the Greek coastal areas (~68%) are phosphorus limited (P- Limited), while ~30% are nitrogen limited (N-limited) and only 2% of the studied coastal areas reveal Si-limitation. However, a shift from P-limitation to N-limitations is recorded during summer period. More than 50% of the Greek coastal areas with N-limitation are classified into Poor, Bad and Moderate trophic status, based on the chl-a classification system, whereas the majority of the Greek areas revealing P- limitation are classified into High and Good status. Moreover, the N-limited areas are affected mainly by sewage discharges, nutrient inputs from river discharges and aquaculture activities. Phosphate content seems to be the most important parameter affecting the functioning of the P- limited areas, whereas, at stations with relatively lower DIN:P ratio, the nitrate to ammonium ratio is really important.

This work was performed under the Water Framework Directive (WFD) implementation within the framework of the National Monitoring Project of Greece.

[1] Glibert P. M. (2012). Ecological stoichiometry and its implications for aquatic ecosystem sustainability. Current Opinion in Environmental Sustainability, 4: 272–277; [2] Pavlidou et al., (2015). Methods of eutrophication assessment in the context of the water framework directive: Examples from the Eastern Mediterranean coastal areas, Continental Shelf Research, 108: 156-168; [3] Simboura et al., (2005). A synthesis of the biological quality elements for the implementation of the European Water Framework Directive in the Mediterranean ecoregion: the case of Saronikos Gulf. Ecol. Indic. 5: 253–266.

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Notes

OP 3

In Situ Measurement of Trace Elements in Marine Sediment and Macroalgae by Field Portable-X-ray Fluorescence Spectrometry

Andrew Turner; Murray Brown; Alex Taylor; Hiu Poon

With the miniaturisation of x-ray sources and improvements in fundamental parameters algorithms, field portable-x-ray fluorescence (FP-XRF) is gaining increasing use and application in situ. In this presentation, the novel, in situ use of FP-XRF to measure trace elements (As, Ba, Br, Cu, Fe, Pb, V, Zn) in marine and estuarine sediments and macroalgae is described. The instrument is fitted nose upwards into a portable test stand and connected to a laptop, with samples counted in the shielded well of the stand. Wet sediments of a few g and contained by a polyethylene specimen bag are analysed in a conventional “soils” mode, with detection limits for a 60 second counting period of down to a few ppm for As, Br, Pb and Zn. After correction for water content, elemental concentrations are within 25% of concentrations returned after re-analysis of sediments in the dry state, suggesting that the presence of water has little impact on the absorption of primary or secondary x-rays. After blotting dry external water, sections of macroalgae (*Fucus* and *Ulva*) placed directly over the test stand well are counted for 90 seconds in a “plastics” mode coupled with a thickness correction algorithm configured for the analysis of low density materials. Detection limits of a few ppm are achieved for As, Br and Zn and, after correction for water content, elemental concentrations returned by the XRF correlate significantly, but with varying slopes, with concentrations delivered by ICP-MS following digestion in boiling nitric acid. The use of the method for the rapid, spatial screening of marine sediments and macroalgae is discussed.

The study was funded by A Plymouth University Marine Institute HEIF V grant.

Notes

OP 4

New Insight in Biodegradation Assessment of Oxidized HDPE Oligomers

Anne-Marie Delort; B. Eyheraguibel; M. Traikia,; S. Fontanella; M. Sancelme1; S. Bonhomme; D. Fromageot; J. Lemaire; G. Lauranson; J. Lacoste

Polymer applications have become such essential in our daily life that it is unlikely to think of the suppression of plastic use as a feasible solution in many industrial fields. It is however clear that increasing anthropogenic activities and the omnipresence of polymers greatly contribute to environmental pollution . Oxo-biodegradable polymers were mainly created to improve and replace polymers in single use applications such as plastic bags, packaging or mulching films. Their capacity of fragmentation and biodegradation appeared as a good alternative to limit the resilience of polymers and their impact on the environment but their use as environmentally friendly material is still under debate. While the oxidation processes and the mechanisms leading to fragmentation of oxobiodegradable polyethylene are well known for years, there is still a lack of knowledge on the mechanisms occurring in the biodegradation processes. To understand these processes it is needed to better cahracterize the size and molecular strucures of these oligomers.

The objective of this work was to develop a new approach to assess the specificity and the efficiency of biodegradation of oxidized oligomers extracted from aged HPDE polyethylene films and to bring insight on the mechanisms occurring during biodegradation. ^{1}H NMR spectroscopy and LC Orbitrap™ mass spectrometry were combined together with data processing using Kendrick mass defect calculation and Van Krevelen Diagram.

We showed that the molecular weight of extracted oligomers was lower than 850 Daltons with maximum chain length of 55 carbons. The oligomers were divided into 11 classes of molecules with different oxidation state ranging from 0 to 10. All classes included series of chemically related compounds including up to 19 molecules. 95% of the soluble oligomers were assimilated by a strain of *Rhodococcus rhodocchrous* after 240 days of incubation. Large highly oxidized molecules completely disappeared while the other classes of molecules were still represented. Molecules containing 0-1 oxygen were less degraded. A strong shift to smaller molecules (In conclusion, this work opens new direction of research. First this new approach combining NMR and LC-MS Orbitrap™ together with Kendrick analysis of the data and Van Krevelen diagrams can be used in the future to analyze the structure of oligomers issued from other polymers and also to assess their biodegradability. Second our work brings new insight in biodegradation processes of oxidized HDPE oligomers.

The authors acknowledge Martin Leremboure (ICCF, Clermont-Ferrand) and Bernard Lyan (INRA, Theix) for their technical help and advice and for performing the LC-MS Orbitrap™ measurements. The authors also acknowledge the financial support of European union's FEDER and the Region Auvergne.

Notes

OP 5

A New Method for Measuring the Steady State Concentration of Hydroxyl Radicals in Atmospheric Waters

Audrey Lallement; V. Vinatier ; A. M. Delort ; G. Mailhot

Current global warming is set to increase Earth's temperature and raise sea levels. Parameters that can offset this warming are few and one of the main unknowns is the interaction of clouds and aerosols. Clouds are multiphasic systems including gas, solid and liquid phases. One of the most important molecules that controls cloud water reactivity is the hydroxyl radical, called the detergent of the atmosphere. Its main sources are well known: hydrogen peroxide, nitrite and nitrate photolysis, iron via ligand-to-metal charge-transfer reactions or photo-Fenton chemistry and gas to aqueous phase partitioning of $HO^\bullet$ or O_3 (A. Bianco et al., 2015). Its main sink is dissolved organic matter (T. Arakaki et al., 2013). Until now, the latest hydroxyl radical concentrations were estimated through model simulations and ranged from 10^{-12} to 10^{-16} M. To our knowledge, only one publication did a real measurement of steady state radical hydroxyl concentration in fog waters and one sample of cloud water. For that purpose, they used benzene as a probe, however benzene is now forbidden in European laboratories because of its toxicity (C. Anastasio and K. G. McGregor, 2001). Moreover, the detection was principally performed by HPLC, which is time and cost effective. The main objective of this work is to develop a fast and convenient method with a non-toxic probe to measure the steady state concentration of $HO^\bullet$ in real cloud waters and to evaluate the effect of microorganisms on this concentration.

Here, we used terephthalic acid (TA) as a probe which, reacting with $HO^\bullet$, allows easy detection via the formation of a fluorescent product: 2-hydroxyterephthalic acid. The measurement of TAOH formation rate allowed to calculate $[HO^\bullet]_{SS}$ concentration using the following equation:

$$\frac{d\left[HO^\bullet\right]_{SS}}{dt} = Rf_{HO^\bullet} - k_{TA}.\left[TA\right].\left[HO^\bullet\right]_{SS} - \sum k_{Si}.\left[Si\right].\left[HO^\bullet\right]_{SS} - k_{HO^\bullet}.\left[HO^\bullet\right]_{SS}^2$$

Where $Rf_{HO^\bullet}$ is $HO^\bullet$ formation rate, $k_{TA}\cdot[TA].\left[HO^\bullet\right]_{SS}$ is $[HO^\bullet]$ trapped by TA, $\sum k_{Si}\cdot[Si].\left[HO^\bullet\right]_{SS}$ is $[HO^\bullet]$ trapped by scavengers (Si) (with k_{Si} the second order rate constant between chemical compounds and $HO^\bullet$) and $k_{HO^\bullet}\cdot\left[HO^\bullet\right]_{SS}^2$ is $[HO^\bullet]$ involved in the recombination process. The non-toxicity of the probe was established and incubations of model microbial strains (isolated from cloud) were done in artificial media mimicking marine cloud water (with solar light, hydrogen peroxyde with or without complexed iron as $HO^\bullet$ sources and controlled temperature). Then it was applied for analysis of atmospheric waters: rain and cloud waters from the puy-de-Dôme station (L. Deguilllaume, 2014). The experiments were performed with no treatment of atmospheric waters and after filtration (without microorganisms) allowing us to measure the effect of the native microflora.

In conclusion, we obtained an efficient and rapid method with a non-toxic probe allowing us to measure the concentration of hydroxyl radical at steady state and assess the impact of the microorganisms on it. In atmospheric waters, this concentration is of 10^{-16} M order of magnitude.

We acknowledge the Observatoire de Physique du Globe de Clermont-Ferrand for puy-de-Dôme station access; the ANR (BIOCAP and the region Auvergne-Rhône Alpes for their financial support.

[1] Anastasio, K. G. McGregor. Chemistry of fog waters in California's Central Valley: 1. In situ photoformation of hydroxyl radical and singlet molecular oxygen. Atmos. Environ. 2001, 35, 1079–1089; [2] Arakaki et al., A general scavenging rate constant for reaction of hydroxyl radical with organic carbon in atmospheric waters. Environ. Sci. Technol. 2013, 47, 8196–8203. [3] Bianco et al., A better understanding of hydroxyl radical photochemical sources in cloud waters collected at the puy de Dôme station: experimental vs. modeled formation rates. Atmos. Chem. Phys. 2015, 15, 13923–13955; [4] Deguillaume et al., Classification of clouds sampled at the puy de Dôme (France) based on 10 years of monitoring of their physicochemical properties. Atmos. Chem. Phys., 2014, 1485–1506.

Notes

OP 6

Preliminary Analysis of Organic Pollutants in the Water of Lake Vrutci, Serbia

Branimir Jovančićević; Marija Stešević; Nevena Baltić; Tatjana Šolević; Nevena Baltić, Tatjana Šolević Knudsen

Lake Vrutci is an artificial reservoir lake in western Serbia, close to the city of Uzice. This dammed reservoir was created with a view to protect from floods, retain river deposits and to supply Uzice and its surroundings with water. The objective of this research was a preliminary analysis of organic pollutants in the water of Lake Vrutci. The water samples from this lake were taken in September 2015, from 14 sampling spots. Each sample was extracted using three different methods: liquid-liquid extraction, solid phase extraction and stir bar extraction. The extracts were analyzed using gas chromatography – mass spectrometry (GC-MS), gas chromatography with flame ionization detector (GC-FID) and gas chromatography with electron capture detector (GC-ECD).

GC-MS and GC-FID analyses indicated absence of any organic contaminants in these samples. However, more sensitive GC-ECD analysis showed presence of some pesticides and herbicides in the extracts analyzed. The compounds indentified were: heptachlor, endosulfan I, endosulfan II, DDT, aldrin, lindane, atrazine, propachlor, alachlor, metolachlor, chloroneb, chlorobenzilate and *cis*-permethrin. It can be concluded that, although all these compounds were indentified in the concentrations below the limit of detection of the GC-MS and GC-FID systems used, their identification in the waters of Lake Vrutci points that the monitoring of the water quality at this location is needed in the future.

Notes

OP 7

Environmental Forensics Analysis of Coal Tar DNAPL using GCxGC-TOFMS

Christopher Gallacher; Robert Kalin; Russell Thomas; Richard Lord

The applications for GCxGC-TOFMS to environmental forensic analysis are far reaching and can provide important information from both a legal and remedial standpoint. The wider range of compounds that can be identified within samples increases the probability of identifying unique compounds for use in legal proceedings. The wider range of compounds also helps to inform remediation works and to identify the potential risks associated with a sample. Several case studies will be presented in order to demonstrate the power of GCxGC-TOFS, when combined with multivariate statistics such as PCA and HCA, for the identification of coal tars as well as identification of the production processed used during the manufactured gas process. The methods developed can easily be transferred to the analysis of other environmental samples such as oil and oil contaminated soils.

We thank the Scottish Funding Council (SFC) Glasgow Research Partnership in Engineering, the University of Strathclyde, Parsons Brinckerhoff and National Grid property for funding support.

Notes

OP 8

Circles in the Sand – Assessing the Seasonal Fingerprint of Musks and Siloxanes at the Beach

Daniela Capela; Inês Magalhães; Lúcia Santos; Arminda Alves; Vera Homem

Synthetic musks (SMs) and volatile methylsiloxanes (VMSs) are significant classes of ingredients incorporated in personal care products. SMs are incorporated due to their due to their pleasant odour, while VMSs due to their high thermal stability and smooth texture (Horii and Kannan, 2008). They are extremely used in the formulation of a wide range of cosmetics and personal care products, including creams, lotions, shampoos and also sunscreens. Thus, both SMs and VMSs represent a considerable source of exposure for both humans and environment (Homem et al., 2015; Capela et al., 2016). And although they are incorporated in such products, there are studies that report toxic effects produced by siloxanes in laboratory tests with animals (Quinn et al., 2007). The exposure to SMs revealed carcinogenicity, impairment of fertility and photoallergenicity. Since SMs and VMSs have a widespread use in daily life, they have already been detected in different environmental compartments as biota, aquatic media, air, sediment and soil. Therefore, their ubiquitous occurrence, bioaccumulation and toxic potential, make them compounds of concern for both environmental and human health.

The main aim of the present research was to investigate the application of a quick, easy, cheap, effective, rugged and safe extraction methodology (QuEChERS) coupled to gas chromatography – mass spectrometry (GC-MS) analysis to the determination of SMs and VMSs (linear and cyclic) in beach sands, to characterize their residues in this matrix and to understand their distribution in the Oporto coastal area.

For this purpose, two different QuEChERS methods were used. A previously methodology developed in our research group (Homem et al., 2014) was used to determine SMs and later, it was adapted and optimised to guarantee the best conditions for the VMSs extraction from beach sand. Forty-six sand samples were analysed from 23 beaches located in Porto's metropolitan area in two sampling campaigns (Summer/Winter). Low detection limits and high recoveries (>80%) were determined for both classes of compounds. Tonalide, exaltolide, galaxolide and cyclic VMSs were the most frequently detected compounds. Both SMs and VMSs were found in higher concentrations in the samples from summer campaign. This suggests that the afflux of many tourists to the beaches, using several siloxane and musks-containing products (sun blocks, etc.) can be a decisive input of these chemicals in the summer season in coastal areas.

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Notes

OP 9

Quantum Chemical Modeling of the Formation of OCS From Thiols, DMS, and Polysulfides in the Ocean

<u>Daniela Trogolo</u>; Davide Vione; J. Samuel Arey

We investigated the molecular pathways that lead from reactions of CO with thiols, dimethylsulfide, and polysulfides to the formation of carbonyl sulfide (OCS) in seawater[1]. The oceans are a major source of atmospheric OCS, most likely produced from photochemical and non-photochemical transformations of sulfur-containing species in surface seawater. However, the combination(s) of precursors, reactive species, and mechanisms that contribute the main formation pathways of oceanic OCS remain relatively unexplored. Hypothesized radical and anionic molecular mechanisms involving biogenic thiols, dimethylsulfide, polysulfides, and CO were explored using quantum chemical models. To investigate these pathways, aqueous Gibbs free energies of reaction and kinetic rate constants were determined with density functional theory electronic structure methods. M06-2X functional[2] was employed to optimize the molecular geometries of the species involved in the mechanism and to compute the thermal contribution to the Gibbs free energies for each species, whereas B2PLYPD functional[3,4] was applied to obtain more reliable electronic energies. All reactions considered here take place in water, and the aqueous solvent can interact with the solutes, thereby influencing the thermodynamics and kinetics of the reactions. To account for solvent effects, all reactions were simulated with the implicit solvent model SMD.

Based on quantum chemical models, thiyl radicals, which can be produced from the oxidation of thiolates or from the bond cleavage of dimethylsulfide, are key intermediates that lead to OCS formation in seawater. Cysteine, methanethiol, 3-mercaptopropionic acid, and glutathione are found to be partially responsible for the oceanic OCS. Sulfide and polysulfide species such as HS^*, S^{*-}, S_2^-, and S_2^{2-} can be involved in the formation of OCS in surface ocean as well.

To investigate the role of the photo-produced species, OH^*, $^1O_2$, CO_3^{*-}, and $Br_2^{*}{}_{-}$ in the oxidation of dimethylsulfide, methionine, cysteine, and glutathione, we conducted simulations of coupled photochemistry and reaction kinetics with the APEX model.[5] The results indicate that Br_2^{*-} is expected to play the main role in the photochemical transformation of sulfur-containing species in seawater. The results of the study have broad implications for our understanding of the role of OCS in ocean biogeochemistry and climate.

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Notes

OP 10

Fenton, Photo-fenton and Fenton-like Reactions Triggered by Magnetic Materials

Davide Vione; Marco Minella; Claudio Minero; Khalil Hanna

The (photo-)Fenton process is based on Fe(II) and H_2O_2 to produce oxidizing species (most notably, but not exclusively, the hydroxyl radical) and can be used for water, wastewater and groundwater decontamination [1]. The two reactants can be provided as such or generated photochemically, electrochemically or sonochemically from several precursors, giving rise to many Fenton variants. Use of other metals or peroxides produces the vast Fenton-like family [2].

A major drawback of classical Fenton process is that Fe(II) + H_2O_2 yields Fe(III), insoluble at the ~neutral pH at which treated water is used or discharged, giving a slurry as process waste. The use of ligands to keep Fe(III) dissolved is an option [3], but residual dissolved Fe could easily exceed the water quality requirements and, in this case, a precipitation step would still be needed. An alternative is the use of solid and Fenton-active Fe-containing materials, which provide a low amount of dissolved Fe(II) for Fenton operation and can be recycled for further reaction cycles. Solid recovery is easier with magnetic materials such as magnetite (Fe_3O_4) and Fe° (ZVI: zero-valent iron). This work describes the use of magnetite and ZVI in (photo-)Fenton and (photo-)Fenton-like processes.

Nanometric magnetite undergoes easy surface oxidation to Fe(III) and is often inactive in the dark Fenton process, but it can be activated by UV irradiation. In this case, one can produce $^\circ OH$ radicals with $Fe_3O_4 + H_2O_2$ + UV [4], and $SO_4^{-\circ}$ radicals with $Fe_3O_4 + S_2O_8^{2-}$ + UV [5]. The latter process yields $SO_4^{-\circ}$ that is a more selective oxidant than $^\circ OH$ and can often achieve decontamination with limited interference from dissolved organic matter [2]. Non-stoichiometric magnetite, with a Fe(II) excess in the inner lattice is to be preferred over stoichiometric Fe_3O_4 because of its much higher activity. ZVI + H_2O_2 triggers a dark Fenton reaction with the possibility to use passivated ZVI, which is an spent residual (waste) of the ZVI-based reductive decontamination of e.g. chlorinated hydrocarbons. One can for instance achieve further oxidative degradation of dechlorinated compounds by just adding H_2O_2 to the residues of the dechlorination step.

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Notes

OP 11

Synthesis and Characterization of Cellulose Nanofiber (CNF) and its Sorption Study with Lead (Pb)

Emmanuel Abu-Danso; Amit Bhatnagar; Sirpa Peräniemi; Helena Vepsäläinen; Jouko Vepsäläinen

Nanofibers from biopolymers are gaining wide interest in water treatment applications due to their high mechanical properties, greater specific surface area, versatile surface chemistry and natural abundance. In this work, cellulose nanofibers (CNFs) were synthesized using simple dissolution with alkali-urea-thiourea at below zero temperature from dewaxed cotton (precursor) under optimized conditions. The synthesized CNF and its precursor have been analyzed by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM). The FTIR analysis of CNF revealed the existence of different functional groups which are believed to be responsible for the lead adsorption. Batch experiments were conducted to investigate effect of contact time on lead adsorption by CNF. Preliminary results revealed that adsorption kinetics was fast and adsorption equilibrium was reached in 60 minutes with an adsorbent dose of 5 mg/L and 50 ppm initial lead concentration. The results of this study showed that the highest removal efficiency (> 90%) was achieved with an adsorbent dose of 5 mg/L, contact time of 60 min, initial lead concentration of 50 mg/l and at temperature 25°C. Different kinetic models viz. pseudo-first-order, pseudo-second-order and intraparticle diffusion models were examined to describe the adsorption kinetics. The results of this study showed that CNFs had high potential to adsorb lead from aqueous solutions.

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Notes

OP 12

Impact of Hydroxyl and Sulfate Radicals on the Disinfection Efficiency of Water

Gilles Mailhot; Angelica Bianco; Inmaculada Polo−Lopez; Pilar Fernandez-Ibanez; Marcello Brigante

Water deficiency and water pollution are serious global problems because they limit the access to clean fresh water and they are associated to health risk [1]. For these reasons, water disinfection and reuse is looked-for and treatments to ensure this need must be developed. Among the possible treatments, advanced oxidation processes (AOPs) were studied [2]. These processes produce in situ transitory species, such as hydroxyl radicals ($HO^\bullet$) ($E_0 = 2.80$ V) [3], which can oxidize many organic compounds and can inactivate a wide range of microorganisms. The disinfecting capability of these processes is well known [4]. A new radical−based oxidative process, involving the activation of persulfate ($S_2O_8^{2-}$) ($E_0 = 2.01$ V) to generate the strongly oxidizing sulfate radical anions ($SO_4^{\bullet -}$) ($E_0(SO_4^{\bullet -}/SO4^{2-}) = 2.43$ V) [5], was recently proposed for the treatment of organic pollutants. Persulfate activation leads to the formation of $SO_4^{\bullet -}$, which react with organic compounds with a second order rate constant of the same order than the rate constant obtained with hydroxyl radical.

In the present work the impact of $HO^\bullet$ and $SO_4^{\bullet -}$, produced by photo-Fenton process from Fe(III)EDDS complex in the presence of either H_2O_2 or $S_2O_8^{2-}$ on the inactivation of *Enterococcus Faecalis* in water, was studied and compared. The use of Fe(III)EDDS complexes maintains iron in the soluble form until slightly basic pH and so the photolysis is efficient in a large range of pH, compatible with natural waters. *Enterococcus faecalis* was proposed as an alternative model microorganism because of its higher resistance than *E. coli*, and its inactivation was investigated applying AOPs. Our results show that the concentration of Fe(III)EDDS complex is a key parameter, Fe(III)EDDS complex playing a dual role for the inactivation of microorganisms. Moreover, for the direct application in natural waters, the efficiency in the presence of ubiquitous inorganic compounds, such as carbonate and chloride ions, was investigated. The impact of the different parameters controlling the efficiency of such processes was evaluated and results show a slowdown or an enhancement of disinfection efficiency in the presence of chloride and carbonate ions.

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Notes

OP 13

The Analysis of Natural and Synthetic Estrogens at Sub ppt Levels in Surface Water and Crude Influent Water with the 2D-LC-MS/MS

Guy Wilson; Angela Boad; Hamish Todd; Neil Gatward; Euan Ross

Estrogens are routinely used either as contraceptive medicines or in hormone replacement therapy and can enter aquatic environments via the discharge of final effluent waters. Estrogens are believed to have a negative effect on aquatic environments by disrupting the hormonal systems of fish. In the recent EU directive 2013/39/EU fifteen additional priority substances were added to the water framework directive (2000/60/EC). In this recent update, 17á-ethinylestradiol and 17β-estradiol were not included in this list but instead added to a watch list in order to gather further data regarding the presence of these compounds in aquatic environments and the risks they pose. In this presentation, we describe the analysis of 17β-estradiol, estrone and 17á-ethinylestradiol, in surface and final effluent waters utilizing an off line Oasis HLB and Sep-Pak Silica solid phase extraction, followed by analysis on a 2D ACQUITY UPLC coupled with the XEVO TQ-S tandem quadrupole mass spectrometer.

Notes

OP 14

Hydrocarbon Geochemistry in the Sediments of Aegean sea (Eastern Mediterranean)

Ioannis Hatzianestis; Kostas Parinos; Styliani Chourdaki, Elvira Plakidi

Hydrocarbons are ubiquitous constituents in marine sediments, usually occurring as very complex mixtures. They derive from a variety of allochthonous or autochthonous sources, including terrestrial plants, marine phytoplankton and bacteria, biomass combustion and diagenetic transformation of biogenic precursors. Aliphatic hydrocarbons are also major components of petroleum and all fossil fuels and their presence in the marine environment is strongly associated with petroleum related pollution. On the other hand, polycyclic aromatic hydrocarbons, mostly coming from anthropogenic activities, have been recognized as hazardous environmental chemicals and are included in priority pollutant lists. In this study the distribution, composition and sources of hydrocarbon mixtures were investigated in the sediments of the Aegean Sea, by using a molecular marker approach and several diagnostic criteria and indices. The Aegean sea is a dynamically active area with unique physiographic and hydrodynamical characteristics and is generally characterized by well oxygenated waters and low primary productivity. Surface sediment samples were collected during 2014 from various open sea and coastal stations and the aliphatic and polycyclic aromatic hydrocarbons were determined by GC-MS after Soxhlet extraction and clean-up and fractionation by silica column chromatography.

The highest contamination from aliphatic hydrocarbons (values well above 1000 μg/g) related with petroleum inputs was recorded in marine areas directly influenced from the cities of Athens and Thessaloniki. In open sea and in coastal stations not affected by land based anthropogenic activities aliphatic hydrocarbon concentrations were generally slightly higher than those expected for unpolutted sediments, whereas their molecular profile (the unresolved complex mixture (UCM), C_{27}-C_{35} hopanes and the CPI values of n-alkanes) indicated a slight chronic oil pollution related to both atmospheric transportation and deposition of hydrocarbons and to merchant shipping and oil transportation. Terrestrial - biogenic inputs were also identified in some areas.

Regarding the polycyclic aromatic hydrocarbons (PAH) several hot-spots across the coastal zone were identified, related to local pollution sources. The study of PAH compositional profiles (parent compound and alkyl homologue distributions, specific isomeric compound ratios) revealed a dominant pyrolytic origin of PAH in almost all the sites examined, while the petrogenic inputs were less important. With respect to the ecotoxicological effects, a high probability of toxicity for the marine organisms was found only in 2% of the samples examined and it was mostly related to coastal industrial activities.

Notes

OP 15

How to Characterize Different Polymer Types in Micro Plastic Polluted Soil or Sediment Samples

Jan Schwarzbauer; Johannes Scherr

Micro plastics are emerging pollutants in the aquatic environment currently attracting a high scientific attention (e.g. Andrady 2011). Beside their possible harmful impact on ecosystems the analyses of such particulate polymers in natural samples is a huge challenge for analysts. So far, a separation based on the different densities of micro plastics and soil or sediment material is the initial analytical step. Following, particles are counted or investigated dominantly by microscopy. As a result the particle concentration can be obtained, but information on the type of polymer is often not available. To a very low extent spectroscopic methods are used in order to chemically characterize micro plastic, e.g. µ-Raman spectroscopy. However, these approaches are rarely reported (Song et al. 2015) and do not allow to quantify the proportion of micro plastic in natural samples.

Here we report on two complementary approaches overcoming the two constraints of analytical approaches used so far for micro plastic analyses in soils or sediments. Based on µFTIR a systematic differentiation of most common polymers (e.g. PP. PET, PMMA, PVC etc.) can be achieved for particles down to 10 µm. Here, sample preparation for microscopy is used that enables a measurement of the total sample without any separation steps. In combination, online-pyrolysis coupled with GC/MS allows the identification of polymers based on their specific pyrolysis products. External calibration of these specific products can be used for quantification. However, as limiting factor a separation of plastic particles from soil or sediment samples with high organic matter content is necessary due to a superimposition of pyrolysis products from natural organic macromolecular matter. Several examples of application and results from both analytical methods applied complementary will be presented and discussed.

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Notes

OP 16

Experience with Online Monitoring of Municipal Wastewater Treatment Plant

Josef Caslavsky; Jiri Marek; Michal Petrulak; Ondrej Dolezal

Wastewater treatment sector is dynamically changing under the influence of new technologies and capabilities of information and communication technologies. The overall concept of Wastewater Treatment Facilities (WWTPs) is moving towards the concept of Water Resource Recovery Facilities (WRRFs) and topics like "water-energy nexus" are becoming a common practise. To be able to practically implement these changes, there is need for more structured and detailed information about the whole treatment process. Thus wastewater monitoring is becoming even more important and the use of new online analytical measurement is every time more and more used.

The presentation is going to discuss practical experience of the use of online analytical sensors for wastewater treatment plant. Authors background is based on our experience gathered from our first pilot plant use (WWTP of approximately 15 000 P.E.) of these sensors and present some ideas, how to use these sensors and data in the future. Based on this, there are also going to be discussed other problems arising from this new approach like data handling, validation of results, calibration etc.

All these new possibilities bring new ideas for the WTTPs operation management. And can bring new insight towards the wastewater treatment of future.

Financial support from the project No. LO1408 "AdMaS UP", from institutional research plan no FCH-S-16-3364, from project Brno Ph.D. Talent and from company SWC InTech Ltd. is greatly acknowledged.

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Notes

OP 17

Analysis of Food Contact Materials using Comprehensive Gas Chromatography in combination with High Resolution Time-of-flight Mass Spectrometry

Alan Griffiths

Food contact materials are materials that are intended to be in contact with food. These can be things that are quite obvious like a glass or a can for soft drinks, but also machinery in a food factory or a coffee machine. Food contact materials can be constructed from a variety of materials like plastics, rubber, paper, coatings, metal etc. In many cases a combination is used; for example a carton box for juices can include (from the inside to the outside): plastic layer, aluminium, paper, printing and top coating. During the contact of the food contact materials with the food, molecules can migrate from the food contact material to the food. Because of this, in many countries regulations are made to ensure food safety. In Europe the framework Regulation (EC) No. 935/2004 [1] applies to all food contact materials. Leachable substances are subdivided into Intent&Listed, Intent&Non-Listed and Non-Intent&Non-Listed.

Especially for the last group (NIAS), established analysis methods using an LC-GC-FID system do not provide enough information. In this study comprehensive two-dimensional gas chromatography (GCXGC) in combination with high resolution time-of-flight mass spectrometry was evaluated.

Beside liquid injections, sample introduction techniques like static/dynamic headspace and thermal desorption were included. A greater amount of information can be gained by pairing an additional complementary separation with two-dimensional gas chromatography (GCxGC). The Consumable Free (CF) LECO GCxGC system takes advantage of a dual-stage, quad-jet thermal modulator positioned between the two columns and a secondary oven allows independent temperature control of the second dimension column. The addition of a high resolution multi-reflecting TOFMS, with a resolving power greater than 25000 (FWHM) and sub ppm mass accuracies, provided accurate mass data adding more confidence in analyte identification. Besides traditional EI ionization chemical ionization (CI positive) was used to confirm the mass to charge ratio of the molecular ion.

The data processing focused on both targeted and non-targeted analysis. Advanced software features like a comparison tool were used to contrast and identify differences between two samples.

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Notes

OP 18

Levels of lead and other toxic elements in blood of indigenous from the Central Chaco-Paraguay

J.F. Facetti [1,2]; *C.Morales* [3]; *V. Mubiana*[4]; *R. Blust*[4]

For more than 20 years, in the Central Chaco, pigeon hunting it has been a successful economic and social activity. In it, native communities are actively involved as personal assistant hunters, and during that period, many individuals of these communities feed on prey collected. In Paraguay, no studies have been done on the influence of the ingestion of lead-based pellets by people. Absorption of inorganic lead in the gastrointestinal tract is influenced by the physiological state of the person exposed (age, fasting, nutritional status relative to iron and calcium, pregnancy), by the physico-chemical characteristics of the ingested material (particle size, solubility, form of lead) and the amount of ingested lead.

The levels of heavy metals such as As, Cd, Cr, Cu, Pb, Zn and the trace element B were determined in whole blood of natives of the Enxet ethnic group in the Central Chaco Paraguay, with a history of consumption of doves over 5 years. The trace element B was analyzed considering the widespread presence of B in soils and groundwater in the Chaco. In this study, blood samples from 23 individuals of different sexes and ages were collected in the post-hunting season and heavy metals and boron were analyzed using ICPMS technique. The pellet surface present “sponges” structures with micro cavities, which allow more surface contact with gastric acid (pH=2), causing increased availability of lead in the body through liberation of $PbCl_2$ (aq.). The lead shells has a short transit through the gastrointestinal tract. Four reference values for lead (mean = 2.76 $\mu g\ L^{-1}$) were obtain from unexposed individuals living in the community. In one individual (5.2% of the sample), the concentration of lead in the blood slightly exceeds the reference value of 10 $\mu g\ L^{-1}$ adopted by several European countries and the USA. All individuals exposed to lead shows levels above the average of those unexposed individuals, but always below the reference value. Low-exposure level were found and their average concentrations in blood were: As: 2,89 $\mu g\ dL^{-1}$; Cd: 0,07 $\mu g\ dL^{-1}$; Cr: 79,7 $\mu g\ dL^{-1}$; Cu 99.4 $\mu g\ dL^{-1}$; Pb: 5,3 $\mu g\ dL^{-1}$; Zn: 743.7 $\mu g\ L^{-1}$; y B: 25,1 $\mu g\ dL^{-1}$. One individual presented a level of Pb at the limit value.

Considering the absence of sources of lead in the environment, the presence of lead in blood above the level of the group not exposed could be linked to the accidental ingestion of lead pellets levels. It is advisable to study biomarkers of these toxic metals both in humans and in the environment, and determine the overall degree of presence of heavy metals in groundwater occurred in crop fields of game ranchers. Given the results, more research should be done to study the presence of heavy metals in people that consume pigeons hunted with lead pellets.

Notes

OP 19

Tandem Ionisation for Enhanced Monitoring of Environmental Contaminants

James Williams; Laura McGregor; Nick Bukowski; Matt Edwards; Steve Smith; Joe Blanch

Time-of-flight mass spectrometry (TOF MS) has made considerable advances in recent years, with the elimination of mass discrimination (crucial for GC couplings), increased sensitivity and compact instrument designs making the technique more amenable. We will explore an advance in TOF MS technology which is set to further increase its applicability.

The term ‘multiplexing’ is used to describe the combination of multiple data streams into a single, comprehensive stream. Multiplexing can be applied to mass spectrometry in a number of ways but, for the purpose of this presentation, we will focus on fast-switching of ionisation energy to collect both hard (70 eV) and soft (10-20 eV) spectra within a single run – deemed ‘tandem ionisation’.

The ion source used in this study enabled soft electron ionisation to be performed with no inherent loss in sensitivity. Multiplexing between ionisation energies allows conventional 70 eV spectra to be obtained for routine identification against commercial libraries, as well as simplified soft EI spectra for enhanced confidence in identification of compounds which exhibit weak molecular ions and/or similar spectra at 70 eV. This technological advances will be demonstrated using the example of environmental contaminants.

Notes

OP 20

Hybrid ZnO-Enzymes Materials for Environmental Remediation

Marco Sarro; P. Calza; E. Laurenti; M. C. Paganini; F. Spina; C. Varese; P. Mallon

Among the organic pollutants, the attention on emerging contaminants is nowadays increasing because of their ubiquitous presence in the environment. Their behavior in the environment is almost unknown and they represent a potential hazard for human health and environment. Moreover, most of them are resistant to the common systems of treatment of wastewater. For these reasons, it is important to search more efficient methods for the abatement of organic pollutants for tertiary treatment.

In the present work, we chose to combine heterogeneous photocatalysis and enzymes, aimed to exploiting the properties of both systems in achieving a higher abatement of pollutants. Heterogeneous photocatalysis is an Advanced Oxidation Process that exploits the characteristics of some solids semiconductors, i.e. TiO_2 or ZnO, for the formation of reactive species, such as $\cdot OH$ and $O_2^{\cdot -}$, which lead to the decomposition of organic and inorganic pollutants. For instance, ZnO is a non-toxic, inexpensive and stable semiconductor oxide and it is considered a suitable alternative to TiO_2 for photocatalytic applications. Doped semiconductor oxides showed a higher photocatalytic activity: in particular, rare earth ion doping can induce an improvement of photo-catalytic efficiency in many kinds of photocatalysts including ZnO. Based on the above considerations, we synthetized pristine ZnO and Ce-ZnO nanoparticles as photocatalysts *via* a hydrothermal method.

Enzyme-mediated oxidative treatment has been investigated as an alternative of many traditional processes to remove toxic and recalcitrant pollutants from wastewater. Among them laccase and peroxidase enzymes have already been used for the abatement of some contaminants. Peroxidase, containing an iron(III)-porphyrin catalytic center, mediates catalytic cycle involves the two-electron reduction of H_2O_2, followed by the one electron oxidation of two substrate molecules. This mechanism allows to the oxidation of organic and inorganic substances. Laccases are glycosylated multicopper oxidases, able to catalyze the electron transfer from a substrate to a molecule of oxygen, which is thereby reduced to water.

We coupled the synthetized zinc oxides with the laccase and the peroxidase enzymes in order to improve the capability of our system to abate the pollutants. To permit the exploitation of photocatalysis to the treatment of polluted waters, the catalyst has to be in a supported form. Besides, we used the electrospinning to prepare self-supported materials. Nanofibers are characterized by a high surface area suitable for catalytic applications and they could be used as support for catalyst nanoparticles.

Firstly, we investigated the activity of our materials using phenol as probe molecule. Then, we apply the best materials to the abatement of some emerging pollutants, namely diclofenac, naproxen, iopamidol, 2,4-dichlorophenol, imidacloprid and bisphenol A. Results showed that when we tested the hybrid systems we obtained a synergic effect due to the presence of both photocatalysts and enzymes. The increased activity is maintained both when working in aqueous phase or in fibers.

Notes

OP 21

Studies on the Dyes Removal Mechanism Catalysed by a Doped Iron Perovskite: The Effect of Temperature

Maria Laura Tummino; Enzo Laurenti; Francesca Deganello; Alessandra Bianco Prevot; Giuliana Magnacca

Mixed oxides with perovskite-type structure are well-known multifunctional materials: they are very versatile since they can be tailored by changing the chemical species involved in the formula, either by doping or by modifying the synthesis method. Herein, a cerium-doped strontium ferrite was prepared and studied. Strontium ferrite ($SrFeO_3$)-based compounds have been already investigated in the literature for application in many fields, especially as sensors [1] and catalysts for energy devices or for the controlled oxidation of pollutants [2.] In most of these cases, high temperatures are necessary to exploit their catalytic activity, but they were also applied in water remediation [3,4] at much lower operating temperatures. In particular, in few previous papers, they were used as photocatalysts for polluted aqueous solutions[3] treatment upon UV-vis or solar light irradiation. Their reactivity, after light excitation, was mainly ascribed to the formation of reactive oxygen species (ROS) which can degrade organic substrates, but a similar behaviour in dark conditions was also reported [4].

In the present work, for the first time, $Sr_{0.85}Ce_{0.15}FeO_3$ oxide was used both as photocatalyst and as catalyst in dark environment, studying in this latter case the effect of the temperature. The compound was prepared by Solution Combustion Synthesis as described in a previous paper [5] and characterized by several techniques (Temperature-time profiles, XRD with Rietveld analysis, N_2 adsorption, ζ potential measurements, SEM, TEM). Catalyst activity tests were performed by studying the degradation rates of Orange II and Rhodamine B, taken as model toxic substances, in the presence of a simulated solar light (for photocatalysis) or at different temperatures in a thermostatic cell. The formation of reactive oxygen species in the different experimental conditions was also investigated by spin-trapping Electron Paramagnetic Resonance technique.

The temperature dependence of $Sr_{0.85}Ce_{0.15}FeO_3$ catalytic behaviour was assessed irrespective to light irradiation. It is worth to notice that temperatures investigated are comprised in a narrow range (25-80°C) and the substrates abatement pathway depends on the excitation source, namely light or temperature.

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Notes

OP 22

Nitrate Removal from Water Uusing Quaternized Hazelnut Shell and Grape Seed

<u>Marija Nujić</u>; Mirna Habuda-Stanić

Nitrogen and phosphorus are emerging pollutants in agricultural and wastewaters. These compounds can cause eutrophication and are the limiting factor of algae growth in most ecosystems. In addition, excessive nitrate intake causes serious health problems in humans. Therefore, the World Health Organization (WHO) stipulated nitrate concentration limit of 50 mg NO_3^-/L.

Several techniques have been used worldwide for nitrate removal from water: reverse osmosis, electrodialysis, adsorption and ion-exchange. Among all above mentioned, ion-exchange is considered to be the one of the simplest and safest method for nitrate removal. In the past years, there has been a growing interest in preparation of ion-exchange resin from agricultural residues. In this research, hazelnut shell and grape seed were used in the preparation of anion exchangers by epichlorohydrin-triethylamine method (ETM method). Batch tests were used to define the efficiency of nitrate removal using modified hazelnut shell (MHS) and grape seed (MGS), i.e. the effects of initial nitrate concentration (10 – 300 mg NO_3^-/L) and solution temperature (25 – 45 °C) were examined. Langmuir, Freundlich and Dubinin-Radushkevich isotherm models were used to study the obtained equilibrium data. The ion exchange efficiency of MHS and MGS were tested in column experiments and results showed that the sorption effect of resin bed sustained well during three sorption/desorption cycles. The results reported that these agricultural residues have the potential to be used as low-cost sorbents for nitrate removal from contaminated waters.

Notes

OP 23

A New Way of Valorization for Bottom Ash from Municipal Waste Incineration: On-site Pilot Tests for Biogas Treatment

Marta Fontseré; Obis Patrick Germain; Hassen Benbelkacem

Concerns on climate change and the deployment of fossil sources push to the urgent development of renewable energies and reuse of materials to decrease greenhouse gases emissions and the use of raw materials. Biogas, a gas rich in methane (CH_4) and carbon dioxide (CO_2) produced by anaerobic digestion of organic matter, is a promising renewable energy source (electricity, heat, fuel). In 2014, the energy production from biogas in the European Union (EU) was estimated at 14.9 Mtoe; 72% from farm digesters, 18% from landfill and 9% from sewage (EurObserv'er, 2015). At the same time, methane in biogas is a powerful greenhouse gas, thus the benefit of its conversion to useful and clean energy. However, biogas contain a variety of trace pollutants, such as toxic hydrogen sulfide (H_2S), which is the cause of gas engine and turbine corrosion and the formation of sulfur dioxide (SO_2). Hence, the elimination of H_2S is absolutely necessary before biogas valorization.

There are various techniques available for H_2S removal from biogas. Adsorption by activated carbon is one of the most common and suitable methods. However, its high operational costs restrain biogas valorization and promote research on inexpensive alternative adsorbents. Giving a second life to waste and by-products for biogas purification seems a promising solution in line with circular economy strategies (Ducom et al., 2009; Gutiérrez Ortiz et al., 2014; Sarperi et al., 2014).

In this sense, we started working on reusing Municipal Solid Waste Incineration (MSWI) Bottom Ash (BA) for H_2S removal from landfill biogas. Indeed, MSWI BA gathers structural and physicochemical characteristics adequate for the adsorption of H_2S. It must be highlighted that bottom ash is produced in enormous quantities every year (near 18 million tons produced in EU in 2014 (CEWEP, 2015)). Partly is used for road construction but a large amount is still stocked in landfills. Therefore, finding an alternative way of valorization seems necessary.

On-site tests with real biogas were performed in a French landfill. The experimental installation consisted in a 10 kg-BA reactor equipped with a biogas monitoring system (CH_4, CO_2, O_2, H_2O, H_2S and temperature of inlet and outlet biogas were continuously measured). The goal of the tests was, at the same time, to evaluate the capacity of BA to eliminate H_2S and to identify the key operational parameters for the further optimization and control of the process. Bottom ash was capable to retain a large amount of sulfur (> 100 g H_2S/kg BA) and proved to be a potential waste for biogas purification. Nevertheless, suitable operational conditions, specially humidity and contact time, showed to be crucial for improving the adsorption capacity of BA.

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Notes

OP 24

Determination of Metal Pollution Sources

Nenad Zarić; Konstantin Ilijević; Ljubiša Stanisavljević; Ivan Gržetić

As anthropogenic influence expends, so does metal pollution. Hence, more areas need to be monitored. This has led to the use of widespread organisms as biomonitors, since they can provide a cheap alternative to traditional monitoring methods. In this study, honeybees (*Apis mellifera*) have been used for the monitoring of metal pollution [1].The aim of this study was to assess sources of Al, Ba, Cd, Co, Cr, Cu, Fe, Mn, Na, Ni, Sr and Zn in the bodies of honeybees. The study was conducted from September of 2013 to September of 2015, in South Banat district in Serbia Samples were mineralized using microwave digestion. Quantitative analysis was done using ICP-OES.

To explore associations and origins of the analyzed elements most common multivariate statistical methods, principal component analysis (PCA) and cluster analysis (CA), were used [2]. PCA is useful in determining the source of analyzed elements [3]. Hierarchical CA was used to further identify the sources of elements based on their chemical properties. The first two components of PCA explain 81.69 % of the total variance, indicating that all analyzed metals were well represented by two components. The first factor is mainly characterized by Co, Cd, Na, Fe, Mn and Zn with loadings of 0.873, 0.839, 0.790, 0.777, 0.777, and 0.764 respectively. To a lesser extent it is also characterized by Cu with loading of 0.672. This factor might be associated with anthropogenic impact, mostly thermal power plants "Kostolac A & B", iron and steel production company "Hesteel Serbia", and traffic. Second factor is characterized mainly by Ca, Al, Mg, and Cr with loadings of 0.900, 0.872, 0.804, and 0.780 respectively. This factor is to a lesser extent associated with Ba, Sr, and Ni with factor loadings of 0.692, 0.688, and 0.677. This factor is associated with natural sources. The results of CA shows two distinct clusters formed. Ba and Sr form a distinct cluster, which is later merged with a larger cluster which contains Ca and Mg, as well as Al and Cr. Ni is also associated with this cluster, but at a larger distance, since it comes in a greater extent from natural sources, but has some anthropogenic sources as well. This first large cluster corresponds to the PCA second factor. In the second large cluster Co and Cd are tightly bound together. They are joint with Cu and Na, and at a further distance with Fe, Zn, and Mn. These results corroborate PCA which showed that these elements come from the same source.

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Notes

OP 25

3D and 4D NMR Experiments for Structural Charaterisation of Peat Natural Organic Matter

Nicholle Bell; Dusan Uhrin; Margaret Graham

Natural organic matter has numerous roles in a diverse range of biogeochemical processes and ecosystem services. However, our understanding of the function of NOM is hindered by our lack of understanding of its molecular make-up. NOM is a complex mixture containing hundreds to thousands of molecules, which cannot be identified using standard analytical techniques such as GC-MS or HPLC. Two high-resolution analytical techniques, Fourier Transform Ion Cyclotron Resonance Mass Spectrometry and Nuclear Magnetic Resonance Spectroscopy are the most promising tools for the task of structural elucidation of complex mixtures. However the complexity of these chromatographically 'inseparable' mixtures interferes with standard protocols used by these techniques.

Here we present a method by which separation and subsequent identification of individual molecules is achieved spectroscopically using a combination of molecular tagging and novel 3D and 4D NMR experiments. Using this methodology, the molecular structures of the aromatic molecules were identified unambiguously for the first time from a NOM sample extracted from a Scottish Peat samples taken from Red Moss Peat Bog in Balerno near Edinburgh.

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Notes

OP 26

Semi-volatile Organic Contaminants Trapped in Environmental Matrices – Methods to Release Them

Nuno Ratola; Vera Homem; José Avelino Silva; Sara Ramos; Lúcia Santos; Arminda Alves

The number of contaminants being released into our environment is endless and obviously pose a multitude of challenges to research scientists. A myriad of different properties and characteristics have an effect on their life cycles, behaviour and patterns. Moreover, all the matrices serving as transport media or sinks for these pollutants hold precious information on the levels of some chemicals, but keep these data trapped in a way that requires sometimes complicated analytical set-ups that need to be constantly improved, in order to obtain better compound resolution and lower limits of detection, keeping the budget and the environmental impact as small as possible.

In fact, the extraction and analysis of environmental matrices (such as vegetation, soil, air, among others) require effective extraction and clean-up procedures to retain the target compounds and eliminate lipid material and other kinds of interfering elements. The development of multi-matrix studies, still scarce in literature (Silva et al., 2015), is an important short-cut to come up with expedite protocols that allow a comprehensive assessment of the presence of numerous contaminants.

In this presentation we review the different protocols our group has developed in the recent years to "release" and quantify the levels of semi-volatile organic contaminants (SVOCs) in diverse sampling media. More classical procedures based on Soxhlet or ultrasonic extraction and clean-up phases like solid-phase extraction (SPE) or gel permeation chromatography (GPC) were employed before quantification by GC-MS, but also new more environmentally approaches such as 'Quick, Easy, Cheap, Effective, Rugged and Safe' (QuEChERS) technique (Prestes et al., 2011) will also be reported. Legacy and emerging compounds were the targets of our studies: brominated flame retardants (BFRs), polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), polycyclic aromatic hydrocarbons (PAHs) as the former and synthetic fragrances (musks) and volatile methyl siloxanes (VMSs) as the latter.

Methods are presented in terms of validation parameters (detection limits, recovery) and some results from field sampling studies. The quantification was always performed using internal standards, mainly deuterated compounds.

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Notes

OP 27

Reducing Pharmaceuticals in the (aquatic) Environment: A Wicked Problem

Ole Pahl; Karin Helwig; Colin Hunter; Joanne Roberts; Moyra McNaughtan

Pharmaceuticals in the Environment (PiE) are an increasingly recognized risk to the quality of surface- and groundwater. This paper describes the work of a trans-disciplinary EU project (noPILLS) that aimed to better understand the complex system of processes and actors that influence the presence of PiE. Clearly, a problem as complex and wide-ranging as that of pharmaceuticals in the aquatic environment cannot be comprehensively explored by a single project. However, noPILLS aimed to provide a unique insight into the problem by first defining the range of factors affecting PiE, together with related points for intervention, and then investigating these interventions in a trans-disciplinary fashion: in developing the concept of a "medicinal chain" (of processes and actors), noPILLS identified potential "levers for intervention" towards the reduction of pharmaceutical ingress into the aquatic environment. In summary, the noPILLS project has shown that:

- Pharmaceutical micropollutants are ubiquitous in the aquatic environment in the project areas, and contribute to environmental effects; A particular risk highlighted by noPILLS is that of antibiotic resistance in the sewerage network
- Regional differences exist in environmental conditions, as can be expected due to macro-geographical influences (landscape, climate etc), but conditions can also vary within regions and in time, with the biggest factors being influx of effluents and dilution in the environment
- People, acting both as consumers / patients and as professionals play an important role in the medicinal chain and need to be involved more in intervention activities
- Strong regional differences exist in factors that are influenced by human behaviour, attitudes, and awareness; most likely this is primarily a result of regional differences in systems (e.g. health system, funding, waste management)
- There appears to be a relatively high level of underlying willingness to 'do the right thing' both by the general public and professionals, which is largely under-utilized due to lack of information, support or means to change behavior
- Technological interventions are effective in reducing some pharmaceutical micropollutants but present their own challenges in terms of monetary and energy costs
- Training, education and awareness raising, together with good stakeholder management and effective communication, are crucial for the success of all forms of intervention.

The project received EU funding as projects 008B (PILLS) and 300J (noPILLS) from funds of the Transnational Territorial Cooperation programme INTERREG IVB NWE; this support is greatly acknowledged.

Notes

OP 28

Aquatic Carbon Export and Water Quality in Relation to Forest to Bog Restoration Management

Paul Gaffney; Mark Taggart; Mark Hancock; Ruth Robinson; Roxane Andersen

Forest to bog restoration is a land management practice where peatlands afforested with non-native conifers are restored to open bog by removing the trees and blocking drainage ditches. This management is carried out with the aim to re-create healthy blanket bog habitat which also functions to sequester atmospheric carbon. In peatland landscapes the loss of dissolved organic carbon (DOC) through water, is an important component of the carbon budget [1]. Forest to bog restoration, which leads to a rise in the water table and decomposition of brash material may therefore affect aquatic carbon export [2]. The rivers receiving blanket bog drainage are of high quality, with low metal, nutrient and sediment concentrations making them important habitats for Atlantic Salmon. Thus it is essential to understand the effect of forest to bog management on water quality of receiving streams and rivers [3].

This project investigates the short term effect (0 -1 year post management), of forest to bog restoration management on water quality and aquatic carbon export. This is achieved by comparing streams from catchments undergoing forest to bog management with control streams in an open bog and afforested catchment. We found increasing aquatic carbon and nutrient concentrations following restoration. We also observed clear seasonal controls on aquatic carbon concentrations and export. Future changes in temperature and storm patterns may therefore impact these processes.

We acknowledge the support of funders for this project; The Royal Society for the Protection of Birds (RSPB) and University of the Highlands and Islands. We also gratefully acknowledge Forestry Commission, Fountains Forestry, Brook Forestry, The Strath Halladale Partnership, A. Mackay and M. Morrison for land access. This project also received support from a MASTS small grant (Marine Alliance for Science and Technology for Scotland).

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Notes

OP 29

Stability of Avobenzone and its Chlorinated Products Under Selected Environmental Conditions

Polonca Trebse; ChengWang; Polonca Trebše; Mojca Bavcon Kralj; Suzana Košenina; Darko Dolenc; Olga V. Polyakova; Albert T. Lebedev; Viatcheslav Artaev

UV filters represent an important group of anthropogenic organic compounds appearing in swimming pool and marine bath waters due to human activity. Quite often they are treated as emerging contaminants. It has been also shown that some of them may decompose when exposed to light by direct photolytic reactions or in the presence of chlorine and chlorinated medium (water pools, sea water). The formation of halogenated byproducts in chlorinated waters is inevitable, especially when UV filters possess phenolic and/or amino moieties.In this work we present our research, focused on pH stability and photostability of chloro-avobenzone and dichloro-avobenzone, two main chlorinated products of avobenzone, UV-A filter, present in the formulation of sunscreens.

Stability of both chlorinated products as well as avobenzone was assessed by exposing water samples to different pHs (4, and 7) in presence of UV A light. The selected pH was achieved by adding hydrochloric acid. During the period of 10 days, the concentrations of solutions were monitored with the HPLC-UV-Vis system and the pH was monitored with a pH meter, Hanna Instruments HI 8417. After 10 days, solutions were extracted by SPE C18 column, and prepared for GC-MS analysis. Photolytic experiments were performed for 6 hours in photoreactor equipped with polychromatic low-pressure mercury lamps (365 nm). Aqueous solutions were irradiated for fixed periods of time and analysed with HPLC-UV-Vis. After irradiation, the solution was extracted by SPE C18 column, and prepared for GC-MS analysis. GC/MS analysis was carried out with high resolution –Pegasus GC-HRT instrument (LECO, USA), allowing for reliable determination of elemental composition and structures of the transformation products.

Results have shown the differences in stability of all three studied compounds in relation of the pH value. At acidic conditions, all three compounds degrade fast with half-lives between 0.60±0.02 day in the case of dichloro-compounds and 1.44±0.14 day in the case of parent one. At neutral conditions, only dichloro- product degrades fast (half-life 0.20±0.01 day), while avobenzone and chloro- product express much higher stability (up to 3.54±0.31day in the case of avobenzone). In the case of photolysis experiments under UV A light, dichloro- product expressed the lowest UV A stability (half-life 0.20±0.01 min), in comparison with avobenzone and chloro- product. Several degradation products have been identified by GC-MS and the degradation pathway has been proposed.

Notes

OP 30

Removal of Pharmaceuticals and Musk Compounds from Wastewater Using Advanced Oxidation Processes

Tereza Švestková; Tomáš Macsek; Michal Úterský; Pavlína Landová; Milada Vávrová; Petr Hlavínek

Wastewater is considered as primary source of the environmental contamination. Requirements for the quality of discharged wastewater are increasingly stricter. New xenobiotics are monitored. Xenobiotics which are stable and poorly biodegradable are a major risk for environment. Due to their bioaccumulation are in all components of environment, also in the food chain.

Major threats are widely used xenobiotics. Pharmaceuticals and fragrances are the most used and significantly represented in wastewater. Millions of Pharmaceutical product packages are used for human and veterinary use every day. Fragrances are used to aromatize the perfumes, detergents or personal care products. Our work is separate it into two parts. In the first part were determined 2 groups of xenobiotics in wastewater which are purified by conventional methods used in wastewater treatment plant (WWTP). In the first monitored group was a linear musk compounds. The second group represented pharmaceuticals of the NSAID, macrolide and sulfonamide antibiotics. Conventional purifying methods for WWTPs are insufficient for elimination of certain xenobiotics. Especially for xenobiotics which are difficult, slowly or impossible to eliminate by conventional (mechanical -biological) methods. Due to these facts we dealt with the possibility of removal xenobiotics by advanced oxidation processes (AOP) in the second part of our work.

Advanced oxidation processes are used to remove of residual contamination of organic pollution as tertiary treatment on WWTPs. These processes are based on the generation and use of highly reactive free hydroxyl radicals. They are able to oxidize difficult oxidizable pollution and therefore to reduce of environmental contamination. Our AOP unit works with ozone, hydrogen peroxide, UV radiation and their combination.

This study has been worked out under the project No. LO1408 "AdMaS UP - Advanced Materials, Structures and Technologies", supported by Ministry of Education, Youth and Sports under the "National Sustainability Programme I" and under the project FCH-S-16-3364 from the Ministry of Education, Youth and Sports of the Czech Republic.

Notes

OP 31

Environmental Screening Techniques with Strongly Extended Polarity – RPLC-HILIC vs. SFC

Thomas Letzel

One determination strategy to observe organic molecules in complex environmental matrices is typically performed with Reversed Phase – High Performance Liquid Chromatography (RPLC) in combination with mass spectrometry (MS). The strength of RPLC is thereby the retention and separation of semi- and nonpolar molecules (i.e. log D>0).

However, polar and very polar compounds (log D Hydrophilic Interaction Liquid Chromatography (HILIC) allows a systematic separation of very polar molecules, is a complementary technique to RPLC and can be coupled with it to an easy, versatile and robust technique.A second, alternative system presented is the supercritical fluid chromatography (SFC) with packed zwitterionic-HILIC-material. It caused last year a sensation for the analysis of both polar and nonpolar compounds.

Results will be shown for target, suspected-target and non-target screening results of organic trace compounds using both systems within surface and waste waters. Several hundred (up to thousands) substances could be characterized. Especially lots of polar molecules were separated and detected for the first time. Furthermore separation properties can be presented and handling tips will be given.

These novel techniques provide fast and highly reproducible separations, combined with precise compound detection and good sensitivity for a wide range of organic molecules.

Notes

OP 32

Exposure to the Ingredients of Personal Care Products – Do They Really Care for Us?

Vera Homem; Daniela Capela; Eduardo Silva; Lúcia Santos; Arminda Alves

Synthetic musks (SMs) and volatile methylsiloxanes (VMSs) are organic compounds incorporated in different formulations of personal care products, including creams and lotions, bathing and hair care products. SMs are used as fragrance additives and fixative compounds and VMSs as emollients/humectants, antifoaming, viscosity-controlling, film formers, antistatic and emulsifying agents (Lassen et al., 2005). Although in the past decades, it was believed that VMSs and SMs were inert (Heberer, 2002), recent studies reported that they may have toxic effects to humans and the environment. In fact, these compounds are suspected of being carcinogenic (namely nitromusks), of causing impaired fertility, liver damage and oestrogen mimicry (Wang et al., 2013). Due to their ubiquitous occurrence, bioaccumulation and toxic potential, both SMs and VMSs are compounds of concern for environmental and human health. Therefore, the main aim of this study was to assess human exposure (dermal and inhalation) to these emerging compounds based on the use of personal care products (Capela et al., 2016; Homem et al. 2015). It was also intended to investigate the "down-the-drain" emissions, taking into account the qualitative/quantitative evaluation of consumer use of SMs and VMSs containing personal care products.

In this work, an analytical methodology based on quick, easy, cheap, effective, rugged and safe (QuEChERS) extraction followed by gas chromatography-mass spectrometry analysis was used to determine 11 SMs (5 nitromusks, 5 polycyclic and 1 macrocyclic) and 8 VMSs (4 linear and 4 cyclic) in different personal care products. These products were chosen according to the usage patterns of the Oporto population (Portugal).

SMs were detected in all analysed samples and VMSs in 96% and their concentrations varied between 0.01 ng/g and 30 mg/g. Higher levels of SMs were found in perfumes, shampoos and body moisturizes, while shampoos and hair conditioners containing the highest concentrations of VMSs. The human daily exposure to both compounds was estimated (maximum around 300 µg/kg bw/day), as well as the release rates of these compounds into the environment through "down-the-drain" practices (3-6 mg/day). Wash-off products were found to represent the most important emission source.

This work was financed by POCI-01-0145-FEDER-006939 – LEPABE and NORTE-01-0145-FEDER-000005 – LEPABE-2-ECO-INNOVATION, by FEDER through COMPETE2020 - POCI and NORTE2020 and FCT (SFRH/BPD/76974/2011).

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Notes

OP 33

Cloud Analysis: Characterization of the Semi-volatile Organic Compounds in the Clouds by GC/HRMS

Viatcheslav Artaev; D. Mazur; O. Polyakova; I. Canet; M. Vaïtilingom; A-M. Delort; S. Pugh; A. Lebedev

Understanding the chemical makeup of clouds is crucial, as clouds participate in the formation and transformation of chemical species, production and consumption of oxidants, droplet activation and growth, transport and deposition of pollutants. A large fraction of the organic compounds present in the clouds has not been characterized so far and this presentation addresses that gap. We have focused this study on the SVOCs composition in the clouds.

Cloud and rain samples were collected at the puy de Dôme station (France, 1465 m) in the period from 2013 through 2016. The samples were filtered and kept frozen at -20°C before MS analysis. Dichloromethane extracts were analyzed with high resolution time-of-flight mass spectrometer Pegasus® GC-HRT (LECO Corporation, USA) in GC and GCxGC modes. The obtained EI mass spectra were used for analytes identification by utilizing high mass accuracy data and the various tools, provided in the instrument's data processing software (ChromaTOF-HRT).

One hundred thirty two individual organic compounds were identified with various levels of reliability in each of the analyzed samples using high mass accuracy EI spectra. The analysis in GCxGC mode has allowed chromatographic separation of closely eluting and coeluting constituents, making analytes identification more reliable. The content of the samples differs from the usual picture expected for cases of water or soil pollution. For example, the levels of concentration of the dibutyl and bis(2-ethylhexyl)phthalates are rather low. Another peculiarity involves complete absence of the chlorinated compounds. We suggest that chlorine is removed from the clouds due to radical atmospheric reactions. More than 90% of the composition is due to oxygen-containing compounds. These results support suggestions of the presence of oxidative condition in the clouds. Phenols, aldehydes, furans, acids were also detected. The quantitative levels of SVOC were measured using internal standards (deuterated PAH) method and estimated as being in the range 0.1-10 ng/ml.

Notes

OP 34

Efficient Filtration of Emerging Pollutants and Effluent Organic Matter by Polycation-Clay Composite Sorbents

Yael Mishael; Itamar Shabtai; Hagay Kohay; Lior Levy

One of the complexities which water technologies face is treating low concentration of emerging micro-pollutants, such as pharmaceuticals, in the presence of dissolved organic matter (DOM), a heterogeneous mixture of relatively large soluble organic compounds. In the current study, new polycation-clay composites based on the adsorption of quaternized poly-4-vinylpyridine to clay were developed and tailored as sorbents for DOM and micro-organic pollutants. Polycation configuration at the adsorbed state, as trains and as loops and tails, was controlled by three parameters 1. solution ionic strength 2. polycation concentration 3. polycation charge density. Composite micro- and nano-structure was characterized by zeta potential, FTIR, X-ray diffraction and thermal gravimetric analyses (TGA). The filtration of DOM from treated wastewater effluent (EfOM) was more efficient by composite columns, approximately 3-fold higher, than by the granulated activated carbon (GAC) columns. We attribute this high removal mainly to electrostatic interaction between the positively charged composites (zeta potential 40 mV) and the negatively charged components of EfOM (zeta potential -20 mV). Although EfOM removal by filtration columns was not affected by polymer loading or configuration, it is reasonable that a loops and tails configuration will be beneficial for the removal of the smaller micro-organic pollutants which are within the size range of polycation loops and tails. Therefore, the removal of pharmaceuticals, diclofenac, gemfibrozil and ibuprofen from tap water or from EfOM by the composites, with a dominant train configuration (Comp Train) or with a dominant loops and tails configuration (Comp L&T), was tested. The removal of the pharmaceuticals from tap water or from EfOM by the Comp L&T was significantly higher than by the Comp Train, even upon normalizing to the polymer loading. The removal by both composites was obviously higher from tap water (EC=0.75) but the reduction in removal from EfOM (EC=1.5) was not dramatic indicating that the interactions of the anionic pharmaceuticals with the composites are not only electrostatic. Furthermore, this degree of reduction in pharmaceutical removal by the Comp L&T was smaller than the degree of reduction by the Comp Train. These results support that a loops a tails configuration offers beneficial binding sites for micro-pollutants.

Notes

OP 35

Sources and Reactivity of C_{60}-fullerenes in the Environment: Preliminary Investigations

Yann Aminot; Josep Sanchís; Marinella Farré; Damià Barceló; James W. Readman

Since their discovery in 1985 by Sir Harold W. Kroto and colleagues, fullerenes have attracted ever-increasing attention and created numerous applications in all fields of chemistry and physicochemistry (optics, electronics, cosmetics, biomedicine…). As engineered nanomaterials, fullerenes are expected to be released into the environment through industrial and urban wastewaters and/or landfills. In addition, incidental formation of C_{60}-fullerenes from combustion sources has recently been established in the exhausts of common fuels [1]. Natural emission pathways have also been hypothesized with various identifications of “fullerene-like” materials in geological samples. As a consequence of their release, C_{60}s have been detected in river water, surface sediments and soils as well as on aerosols from the sea atmosphere [2-4]. After discharge in the environment, the fate of fullerenes is largely unexplored. In water bodies, the hydrophobic fullerenes can form stable aqueous nano-suspensions or adsorb onto particulate matter. Further degradation processes may involve hydroxylation, oxidation or other surface functionalization but remain largely speculative to date. However, the natural occurrence of C_{60}-O derivatives could be of potential concern as their toxicity remains unknown. It has been shown that oxygenated by-products of organic compounds can exhibit much higher toxicity than their parent compounds, e.g. oxygenated polycyclic aromatic hydrocarbons.

In the present work, we developed and validated an analytical method based on LCHRMS for the quantification of trace levels of fullerenes and their major oxidation by-products. We also report for the first time the environmental occurrence of fullerenes and some fullerene-oxides on urban aerosols and in river water. The conditions of formation of these oxidation products were also investigated. Incubation experiments were conducted under environmentally realistic conditions to evaluate the influence of ionic strength, organic matter, pH and exposure to light on the oxidation of C_{60}-fullerenes.

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Notes

Poster Presentations

PP 1

Efficient Removal of Boron from Hyper-saline Wastewater Using Nano-magnetic Chitosan Beads

Akeem Adeyemi Oladipo; Mustafa Gazi

This paper discusses the successful synthesis of nano-magnetic chitosan beads (NMC) for selective recovery of boron from hyper-saline wastewater. The use of most reported boron adsorbents is hindered by selectivity and separation issues notably in the presence of high concentrations of salt. Therefore, the hydroxyl modified NMC beads were found to be a better substitute to the existing boron adsorbents. The adsorbents were characterised by scanning electron microscopy (SEM), and thermal gravimetric analysis (TGA). The thermogravimetric results, BET surface area and vibrating sample magnetometry data confirmed that the NMC is thermally and mechanically stable to withstand deterioration, had a saturation magnetisation of 75.25 emu/g, the surface area of 435 m^2/g and diameter of 150–400 µm. Under optimised hyper-saline conditions, 145.8 mg/g of boron was removed at pH 7.0, and the NMC efficiently showed remarkable selectivity towards boron in the presence of interfering dye molecules. The sorption mechanism is well predicted by the Freundlich isotherm, and the kinetic analysis indicated that the sorption process was successfully fitted with the pseudo-second-order model. Overall, the NMC demonstrates efficacy as high-performance boron selective adsorbent and can be recovered magnetically after spent.

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Notes

PP 2

Fast Pesticide Residue Analysis Using a Novel Benchtop Time-of-Flight Mass Spectrometer

Alan Griffiths

A method was developed to analyze 203 pesticides in less than 9 mins using a new benchtop gas chromatography/mass spectrometer (GC/MS). Pesticide residue analysis remains an important requirement for food and feed, and sample throughput is of high importance for laboratories looking to lower the cost of sample analysis.

A mixture of 203 pesticides (GC Multiresidue Pesticide Standard #1 to #9; Restek) was analyzed on a novel benchtop GC/MS capable of 50 spectra/s with a mass range from m/z 10 to 1500. An analysis typically developed on a 30m 5MS GC column was translated to a 15m x 0.25mm i.d x 0.25 µm d.f (Restek) for high-throughput analysis.

A mixture containing 203 pesticides was analyzed in less than 9 mins. A majority of the components were resolved by chromatography and spectral deconvolution. A food commodity was spiked with a subset of 34 components (GC Multiresidue Pesticide Standard #5) relevant to the commodity to generate a calibration curve from 0.100 to 2000 ppb in matrix. The samples were also fortified with PCB-18, PCB-28, and PCB-52 for use as internal standards. All of the components were detected at the 1.0 ppm level in matrix, with the majority of components detected at 0.100 ppm, with excellent linearity to 2000 ppm. An unfortified sample was used to measure concentrations of these incurred pesticides in the food commodity.

New benchtop GC/MS capable of high-throughput and low level pesticide residue analysis

Notes

PP 3

Characterization of Fruit Tea Beverages with a New Benchtop GC-Time-of-flight Mass Spectrometer

Alan Griffiths[1], *Juergen Wendt*[2]

[1]LECO UK, [2]LECO European Application & Technology Centre, Berlin

Fruit flavored teas (diet and regular) were characterized and compared in a non-targeted way. The precise characterization of the aroma profile is important for beverage producers, because some analytes have known odor properties, that were related to either the fruit or the tea characteristics of the beverage.

HS-SPME was used to collect the volatile and semi-volatile analytes that likely contribute to the aroma and flavor of the beverages. GC paired with TOFMS is an excellent choice for separating and detecting these analytes and a rapid screening method using LECO's Pegasus BT is demonstrated here.

Data processing methods included automated NonTarget Deconvolution™ of the full m/z range data, which offers an additional level of information with mathematical separation to distinguish chromatographic coelutions. These aspects of the analysis provided the ability to identify and quantify numerous individual analytes and discover more about these samples. The LECO Pegasus BT provides a complete aroma profile for every sample, from every run. With this capability, the diet and regular samples were further characterized and compared to each other for similarities and differences. Many of the analytes were present at comparable levels in each sample, but some differences were also observed.

Notes

PP 4

Production of Biosurfactants by *Pseudomonas Aeruginosa san ai* grown on Crude Oil as a Sole Source of Carbon

Ana Medić; Ivanka Karadžić; Ksenija Stojanović

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Even though petroleum is the most exploited and frequently used energy source, it is also one of the major pollutants of soil and groundwater. Bioremediation techniques based on use of microorganisms for crude oil degradation have been developed as an alternative to chemical and physical techniques for cleaning up oil-polluted environments. *Pseudomonas aeruginosa* is well known for its possibility to grow on different sources of carbon and consequently for remediation of oil-polluted sites.

Production of biosurfactants: rhamnolipids-RL and exopolysaccharide-EPS by *Pseudomonas aeruginosa san ai* during the growth on crude oil as a sole carbon source was investigated. The strain *P. aeruginosa san ai* was isolated from industrial mineral metal-cutting oil [1] and it is known for its ability to produce biotechnologically important substances, such as enzymes (lipase, protease) and biosurfactants: rhamnolipid and exopolysaccharide [2], as well to be used for remediation of heavy metal pollution [3]. Production of biosurfactants RL and ESP was determined during growth of P. aeruginosa san ai on PPAS (phosphate-limited proteose peptone–ammonium salt) medium supplemented with crude oil as a sole C-source. Concentrations of RL and EPS were determined by standard methods [4, 5], whereas bacterial growth was monitored as the change of optical density, correlated with number of viable cells.

During its growth on PPAS supplemented with crude oil *P. aeruginosa san ai* produces both biosurfactants. However, production of RL and EPS is relatively low compared with other used C-sources, reaching maximum of 37.4 mg/L for RL and 39.7 mg/L for EPS after 120 hours of growth. Observed growth rate was low but number of viable cells was constant during the stationary phase, suggesting that the strain can use crude oil as a C-source for the biosurfactants production. Slower growth rate and biomass yield can be interpreted as being caused by the chemical composition of crude oil (which contains more than 100 000 of individual compounds, belonging to four basic fractions: saturated hydrocarbons, aromatics, polars and asphaltenes). Such complex mixture is less available to microorganisms and harder to degrade. The results have demonstrated that the strain *P. aeruginosa san ai* can grow on crude oil producing biosurfactants RL and EPS. Thus the strain has a good potential to be applied in bioremediation of environments accidentally polluted by crude oil or products of petroleum industry.

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Notes

PP 5

Geographic Variation in Liver Element Profiles of Wild Red Deer

Andrew French

Red deer (*Cervus elaphus*) naturally accumulate essential trace and toxic elements in liver tissue. Liver element concentrations are associated with plants (soil adhered to those plants, e.g., to roots) and water ingested; and as such, liver element profiles vary between contrasting geochemical landscapes. We explore the extent of this variation in the Scottish Highlands. Liver tissue was collected from the carcasses of wild red deer (male, n = 427; female, n = 343) in nine isolated populations during two hunting seasons (2012-13 and 2013-14). Samples were processed by UV-assisted total acid digestion and analysed by ICP-OES for largely essential trace (Cu, Co, Mn, Se, Fe, Mo, Zn, Ti, Al, Ni), macro (Ca, K, Mg, Na, P, S), and toxic (As, Cd, Hg, Pb) element content. Marked geographic variation in cadmium, copper, molybdenum and selenium concentrations were found between populations, and further overarching distinctions between populations were found using principal component analyses. Females typically had higher essential element status than males (for whom essential element status decreased during the breeding season), and toxic elements were found in greatest concentrations in the oldest animals. Wild red deer essential trace and toxic element status varies markedly in the Scottish Highlands, and the consequence of which may affect sub-clinical health, welfare and performance. Owing to the lack of comparable data in this species, this dataset forms a baseline reference for future studies.

Notes

PP 6

Impact of Atmospheric Stresses on Clouds Microorganism's Metabolome: The Case Study of H_2O_2

Anne-Marie Delort; Nolwenn Wirgot; Marie Lagrée; Martine Sancelme; Mounir Traïkia; Cyril Jousse; Isabelle Canet

In cloud water collected at the puy de Dôme mountain (France), microorganisms are metabolically active and are exposed to very strong stress, especially due to the presence of reactive oxygenated species, including H_2O_2 and radicals. Indeed, cloud water is a very oxidized environment with a redox potential of up to 200 mV (Deguillaume et al., 2014). However cloud microorganisms can survive to oxidative stress (Joly et al., 2015) and are able to degrade H_2O_2 (Vaitilingom et al., 2013). In a recent work, we highlighted that H_2O_2 modulates the global metabolism of cloud microorganisms as shown by strong correlation between ATP concentration (adenosine triphosphate) and the presence of H_2O_2 (Wirgot et al., in prep). We have seen an impact of H_2O_2 in the degradation of carbon compounds present in cloud water samples. The question remains: how do microorganisms resist to these atmospheric stresses, and particularly to the exposure to H_2O_2? How do their metabolome respond to this stress?

To answer to this question, we thought it was appropriate to deepen our knowledge of the interactions between bacteria and H_2O_2 in cloud water by a metabolomic approach. For this purpose we have investigated the response of a *Pseudomonas* strain (a genus frequently found active in cloud water samples) to hydrogen peroxide exposure. Experiments were performed in three biological batches of 12 samples. 24 erlenmeyers flasks were incubated at 17°C and 110 r.p.m containing 150 mL of cloudwater solution and inoculated with bacterial cells close to 107 cells. mL^{-1}. 200 µM of hydrogen peroxide were added in half of them. The experiment was stopped at 50 minutes and 24 hours of incubation because these two different time points are important regarding the evolution of ATP cellular content and H_2O_2 degradation over time. Bacterial pellets were obtained by centrifugation (5 min, 12000 g) and rinsed twice in a 0.8% solution of sodium chloride. Then, they were extracted by a cold water/methanol/acetonitrile mix. 12 samples were obtained for each time point (half submitted to H_2O_2). Finally, we analysed samples via LC/MS and 1H-NMR using the Metabolic Profiler® facility (Bruker). Metabolic profiles were converted into matrices using Galaxy platform and Amix. Statistical analyses (PCA, PLS-DA) were performed with SIMCA-P software. Assignments of biomarkers are in progress.

This research is supported by the ANR program, METABOHUB. Nolwenn WIRGOT is recipient of a PhD grant from the french ministery of research.

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Notes

PP 7

Magnetite-modified Chicken Bone Biochar for Removal of Tetracycline and Fluorescent Dye from Wastewater: Two-stage Stirred Adsorber Design

Ayodeji Olugbenga Ifebajo; Akeem Adeyemi Oladipo

Here, magnetite-modified chicken bone biochar (MCB) was fabricated and characterised. The Brunauer-Emmett-Teller (BET) surface area, magnetisation value and pH_{pzc} of the MCB were found to be 296 m^2g^{-1}, 1.25 emu and 8.3 respectively. The MCB efficiently adsorbed rhodamine B dye (RB) and tetracycline (TC) in a two-stage stirred adsorber (TSA). The TSA reduces the pressure drops, mass transfer resistances, and fouling of the adsorbent. About 89% and 83% of the initial adsorption of RB and TC on the MCB was recorded in a single-stage system using 96.3 g MCB. However, the TSA optimisation studies indicated that 46.5 g of MCB and 120 min are required for the removal of 93.5% and 98.5% of 80 mgL^{-1} of TC and RB from simulated effluent solutions, respectively. The optimised two-stage stirred adsorber system offers higher percentages of removal and shorter treatment times as compared to the single-stage system. The sorption mechanism follows a heterogeneous multilayer chemisorption process. The MCB could be rapidly separated after saturated adsorption by an external magnet, easily regenerated and reused with little sorption capacity loss.

Notes

PP 8

Investigating adsorption capacity of *Delonix regia* for the Removal of Metal Ions from Aqueous Solutions

Bolanle Babalola; Hao Zhang

The adsorption capacity of *Delonix regia* pods was investigated for the removal of cadmium, lead, copper, nickel and cobalt from aqueous solution using batch experiment. The effect of operating parameters such as pH and contact time was studied. Investigation was also carried out by varying the ionic strength and adsorbate concentrations of the aqueous solutions.

The studies revealed that the sorption process of *Delonix regia* for cadmium, lead, copper, nickel and cobalt is highly dependent on pH, contact time, and metal ions concentration in the solution. It also showed that the adsorption capacity decreased with increase in the ionic strength of the solution. The time dependent studies gave a maximum sorption within 30 minutes of contact and a correlation factor greater than 0.999 for all the metals investigated when the data were modelled with the pseudo second order kinetic model, while the Isotherm parameters were best fitted into the Langmiur Isotherm.

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Notes

PP 9

The Occurrence of Sulfur in Late Miocene Lignite from the Kovin Deposit, Serbia

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The purpose of this study was to investigate connection between sulfur enrichment, coal lithotype and mineral content of lignite from the Kovin deposit, Serbia. In coal, major forms of sulfur are organic, pyritic and sulfate sulfur. The bulk of the sulfur in low-sulfur coal and some of the sulfur in medium- and high-sulfur coal is incorporated at the time of peat accumulation. Most coal pyrite and organic sulfur compounds are formed during early diagenesis of coal [1]. The presence of sulfur in coal is important for understanding conditions of depositional environment and for indicating the influence of certain microbes, such as sulfate-reducing bacteria.

Total of the 43 samples divided into 4 main lithotype groups (namely, xylite-rich, stratified matrix, mixture of matrix and xylite-rich and mixture of matrix and mineral-rich coal) were studied. 63 % of samples have total sufur content Stot > 1 % and 14 % have Stot > 3 % which is considered to be medium- to high-sulfur coal [2]. Stot for these 33 samples ranges from 1 % to 4.4 %, averaging at 2.06 %. Both the highest and lowest content of Stot is observed for mixture of matrix and mineral-rich lithotype which could be explained by varying amount of mineral matter input in all 33 samples, 3.3-23.9 %, 11.62 % in average. SEM-EDS examination on Kovin lignite revealed that the most abundant minerals are clays, silicates, sulfate and carbonate, while pyrite is the most abundant sulfide mineral. Relatively significant correlation coefficients between Stot and pyrite, as well as Stot and Fe (r=0.73 and r=0.70, respectively), possibly indicate the same origin and close connection with pyrite. In certain Hungarian Miocene coal from the Pannonian Basin, freshwater inflow and high depositional rates affected the marginal paleoenvironmental location which caused deviation in sulfur content [3].

The variation of sulfur content in coal is controlled by geologic conditions during coal formation. In medium- and high-sulfur coals, seawater is a predominant source of sulfur in the form of sulfate, which is reduced by anaerobic, sulfate-reducing bacteria. Marine influence of Pannonian Sea, which was already converted in Lake Pannon by the time Kovin deposit was being formed (Late Miocene, [4]), slowly and gradually transited to freshwater environment. Unexpected sulfur enrichment for terrestrial coal could to be the remnant from ancient sea environment that influenced peat formation as well as sulfide mineralization.

The study was financed by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project number 176006).

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Notes

PP 10

Siloxanes – WWTP? (Where Will They Persist?)

Daniela Capela; Nuno Ratola; Arminda Alves; Vera Homem

Siloxanes are a subgroup of silicones, containing Si-O bonds with organic groups attached to this backbone (mostly methyl groups). They are widely used in several industrial processes and consumer products such as detergents, personal care products, cosmetics, paper-coatings and textile due to their properties and are moreover feedstock chemicals for the production of silicones (Dewil et al., 2006).

Volatile methylsiloxanes (VMSs) are semi-volatile and due to their lipophilic behaviour they tend to bioaccumulate and persist and also to biomagnify in living organisms. VMSs have also a potentially toxic behaviour, namely the cyclic compounds, being connected to disruption of the endocrine system, connective tissue disorders as well as adverse immunologic responses (Surita et al., 2014).

VMSs have a widespread use in daily life and, therefore, are likely to be released via household effluents, reaching wastewater treatment plants (WWTPs), where they are not completely removed (Whelan et al., 2010). Here, adsorption and volatilization processes play significant and competing roles in their removal. In fact, due to their lipophilic nature, sewage sludge is one important transitional sink and a reservoir that should be of special concern to investigate. Therefore, the use of sludge/biosolids for agricultural purposes may be a direct input of these contaminants into soils. On the other hand, effluent discharges are the major route for surface water and aquatic biota contamination. In short, WWTPs may be considered as crucial emission routes of these contaminants to the environment. So it is essential to assess the occurrence, behaviour/distribution and ecological risks of VMSs in the WWTPs.

Therefore, the main objective of this work is to draw a comprehensive picture of the presence of VMSs in WWTPs, compiling and discussing their occurrence in the sewage, effluents and sludge, main concentration levels and phase distribution and the efficiency of the different methodologies applied in the treatment facilities.

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Notes

PP 11

Annual Variations in Trace Element Levels in the Atmosphere as Detected in Holm Oak Bark of Branch Segments

Daniele Brignole; Drava Giuliana; Giordani Paolo; Minganti Vincenzo

The use of tree parts (leaves, bark, …) as bioindicators for the determination of trace elements is a well-known and established technique. This approach has several advantages: 1) trees are present in all the cities, being exposed to the same atmospheric contaminants as people living in those urban environments; 2) a sufficient number of samples can be easily collected, with a satisfying sampling density; 3) the concentrations of several elements can be determined by means of widely used analytical techniques, with instruments which are commonly available in laboratories. Moreover, the bark of each annual segment of tree branches is exposed to the atmosphere for a known period of time and it is thus possible to reconstruct past changes in trace element deposition, as shown by previous studies performed by our research group.

For this project, branches of holm oak (*Quercus ilex* L.) were sampled in the city of Genoa (Italy) and segments covering the period from 2001 to 2013 were obtained. Samples were collected in an area which is close to industrial settlements (a steel plant and port activities). Arsenic, Cd, Co, Cu, Fe, Mn, Ni, Pb, V and Zn concentrations were measured by atomic emission spectrometry (ICP-OES). The annual variations in trace element concentrations were investigated on the basis of ordinary least squares regression and analysis of residuals. In particular, Cd and Pb show very similar annual variations. In general, the branch segments attributed to 2005 are characterized by high concentrations of most of the elements, except for Cu, Fe and Zn. Another common feature is given by low values in the years 2003 and 2004, except for As, Cu and Mn. The observed variations in trace element concentrations are not correlated with climatic data (mean temperature and rainfall). This approach allows to highlight groups of trace elements showing correspondences in temporal variations.

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Notes

PP 12

Soil Searching in Northern Scotland

David Braidwood; Graeme Morgan; Mark Taggart; Melanie Smith; Roxane Andersen

The Dounreay nuclear plant, a former research centre, on the coast of northern Scotland, is in the process of being decommissioned and demolished. A requirement of this is that during the interim end state (IES), from 2033 - 2333, the area is able to support native vegetation, and that at the final end state (FES) in 2033, the site is available and safe for alternative uses. The areas of the site which have been historically contaminated need to have a one metre remediation layer added at the surface which will prevent contaminants reaching surface vegetation, and ultimately the fauna.

Surveys carried out across the surrounding north coast of Sutherland and Caithness measured the vegetation present, and a classification of the soils from each of the surveyed quadrats was made through laboratory analysis. Parallel to these surveys, vegetation trial plots were set up at Dounreay using a range of treatments including two sizes of crushed rock, below 90 mm and below 35 mm, topsoil, and different seed mixes were sown on these of desired species.

The data have been analysed to find out 1) which soils in the north coast best support the desired vegetation, 2) how comparable soils from the North coast and soil used in the trials are, and 3) what potential limitations could prevent the trial soils to support the vegetation targeted for restoration.

Notes

PP 13

Dynamics of Inorganic Components in Lake Waters from Terra Nova Bay, Antarctica

Eleonora Conca; M. Malandrino; A. Giacomino; S. Buoso; S. Berto ; O. Abollino

Water and Suspended Particulate Material (SPM) samples analyzed in this work were collected in the austral summer 2011/12 from six shallow Antarctic lakes (Carezza, Edmonson Point 14 and 15a, Gondwana, Inexpressible Island 10b and Tarn Flat 20) of Terra Nova Bay (Northern Victoria Land, Antarctica). The total concentrations of a large suite of inorganic analytes were determined, in order to gain insight into the natural processes regulating species distribution, define natural background values and detect possible present or future local and/or global anthropogenic contamination. Lake water composition was found to be influenced by marine spray, lake geographical position and meltwater input. Seasonal variability was also evaluated for every analyte, and explained with regards to its origin. Multivariate chemometric techniques were performed in order to identify groups of samples with similar characteristics and find out similarities and correlations among variables. The variability observed within the water samples is closely connected to the sea spray input; hence, it is primarily a consequence of geographical and meteorological factors, such as distance from the ocean and time of year. Higher element concentrations have been found in SPM than in water, showing that adsorption processes might take place. SPM samples were also observed with a SEM, and many diatoms belonging to different species were found. No evidence of a detectable metal contamination was found in the investigated area.

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Notes

PP 14

Can Marine-derived Plastic Litter Be Used in Water Remediation?

Emily R. Kearl; Mark A. Taggart; Neil A. James; Kenneth G. Boyd; Stuart W. Gibb

Plastic pollution in the marine environment poses a threat to marine ecosystems, giving rise to a multitude of hazards due to entanglement, ingestion by marine organisms and as it provides a vehicle for invasive species. Indirectly, plastics can also act as a source and vector of contaminants to organisms through ingestion (Teuten et al. 2007). Contaminants include components of the plastics themselves (i.e., plasticisers) and also compounds/elements that become adsorbed onto the material from seawater (i.e., heavy metals and hydrophobic organic compounds such as PCBs and PAHs. Can we use this property of plastic to our advantage? The presence of emerging contaminants (i.e., PPCPs and EDCs) in our water resources is of increasing concern. Most conventional water treatment plants were not designed to remove these contaminants efficiently and there currently exists limited legislation requiring and enforcing their removal. This project, linked to the Northern Periphery and Arctic (NPA) programme project "Circular Ocean", assesses the potential for discarded marine plastic (particularly ropes and nets) to be repurposed as a low-cost sorbent material for the removal of contaminants from wastewater streams. Presented here are preliminary data from Pb and Cd sorption tests carried out to compare weathered and new rope material. Sorption kinetics, differences between old and new ropes and differences between types of rope (i.e., polymer concerned) are discussed.

We thank Dagmar Svobodova for guidance in laboratory procedures. This research was funded by UHI and Circular Ocean (funded under the ERDF Interreg VB Northern Periphery and Arctic (NPA) programme).

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Notes

PP 15

Assessment of Impact of Land Cover and Geological Settings on the Soil Physic-chemical Properties in Mountain Region of Fruška Gora (Serbia)

Gordana Gajica; Milica Kašanin-Grubin; Milan Milenković; Aleksandar Lazarević; Srdjan Bojović; Branimir Jovančićević

Globally, land use change is one of the most important issues in the assessment of environmental change, and must be clearly understood for the sake of the ecosystem sustainability. The aim of this study was to determine the influence of land use and geological settings on the physico-chemical properties of soils in the environmentally vulnerable mountainous areas of Fruška Gora (Serbia). Fruška Gora covers an area of 260,000 km^2 and is geologically very diverse in the sense that it is built of rocks of different composition and age. Until World War II Fruška Gora was largely covered with forests (130.000 ha), but now only 25.000 ha is forested area. During this period, land use type has changed in many parts of this mountain and now besides forests, there are agricultural land, vineyards, meadows and urban areas.

For the purposes of this study total of 47 soil samples were analyzed: 23 samples of forest land and 24 samples of meadow land. Geological setting of forest land was serpentinite, limestone, schist and trachyte, and geological setting of meadow was serpentinite, limestone and loess. In all soils samples following parameters were determined: pH, redox potential (Eh), electrical conductivity (EC), available ions (Na^+, K^+, Ca^{2+}, Mg^{2+}), sodium adsorption ratio (SAR), and concentration of organic carbon (Corg).

Statistically significant difference between the analyzed forest and meadow soils was found in the content of Corg and no statistically significant difference in the values of pH, Eh, EC, SAR. Therefore it can be concluded that the two studied vegetation types do not have a significant impact on the soil pH, Eh, EC and the SAR values. On the other hand, the content of Corg to a large extent depends on the vegetation type and land use. Based on EC and SAR ratio tested soils are potentially dispersive, which means that there is no immediate danger of erosion, but severe disturbance could lead to a prominent reaction of land degradation.

The study was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project No. 176006).

Notes

PP 16

Ecotoxicological Evaluation of Energetic Byproducts

Helena Zlamalova Gargosova; Petr Kral

High production of waste belongs to serious global problems. In the Czech Republic during 2012 total amount of 23 171 000 tons of waste was produced, 1 481 000 tons of them was hazardous waste [1]. This could pose increased risk for the environment and human health and thus requires a stricter control regime.

Significant increase in consumption of energy resulted in more intensive use of fossil fuels and fuel derived from renewable energy sources. Power plants produce also energetic by-products (EBPs), mainly ash and desulphurization products, which were primarily considered as waste materials [2]. Thus these can be classified as hazardous or non-hazardous depending on the content of hazardous substances and other risk properties [3]. On the other hand, they could be used as useful material for reclamation purposes etc. if they are safe for the environment.

The topic of our study was evaluation of ecotoxicity of EBP produced by the power industry. Samples of EBPs (Bed ash, Fly ash, Cinders, Product of the desulfurization) were supplied by four different anonymous energy producing companies. Information which had been provided concerned only characterization of fuels used by the power plant. EBP were subjected to ecotoxicological testing via direct contact tests and via testing of water leaches of these samples prepared in accordance with methodology described in valid Czech legislation on waste management. In contact arrangement tests on terrestrial organisms: Acute toxicity test and Avoidance test on soil organism earthworm (*Eisenia fetida*) and Plant root growth inhibition test on letuce and onion (*Lactuca sativa* and *Allium cepa*) were used. Luminescent bacteria test on *Vibrio fischeri* represented tests in aquatic arrangement and serves to testing of water leachates. It was found that tests in contact arrangement are very important for complex evaluation of negative effects of matrices entering the ecosystem. Water leachates from waste often underestimate negative effect of present water-insoluble compounds. Also the importance of test on luminescent bacteria *Vibrio fischeri* is not negligible, because this test provides additional information of effects on representatives of destruents as an important ecosystem function part. Bed ash, fly ash and product of the desulfurization exhibited various ecotoxicity in dependence on fuel composition. On the other hand cinder was almost in all test the least toxic; in some cases exhibits stimulation effects.

This work was supported by the institution research plan No. FCH-S-16-3364 from the Ministry of Education, Youth and Sports of the Czech Republic.

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Notes

PP 17

Green Synthesis of Silver Nanoparticles Using Grape Stalk Waste Extract

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Nowadays, nanotechnology is one of the most active areas of research. Metal nanoparticles exhibit interesting optical, magnetic and catalytic properties that made these nanosized metals useful in many emerging applications. Chemical synthesis of silver nanoparticles has been carried out by using a variety of reducing systems that includes $NaBH_4$, Cu, Ni, Co complexes and macrocyclic ligands. Taking into account that the solvents and the reducing agents used for nanoparticles production are toxic, in the recent years great efforts have been made to find more sustainable methods and less toxic reagents to synthesize nanoparticles. It has been reported that plants possess components that can act as reducing agent and stabilizers in the nanoparticles production.

In this work, the synthesis of silver nanoparticles by reduction of silver ions in an aqueous solution of grape stalk waste extract is presented. Recently, it has been reported that this waste possesses reducing agents like polyphenolic compounds and sugars (Pujol et al. 2013).

The extract containing the reducing agents was obtained by putting into contact the wastes at a given particle size with Milli-Q water. The effect of temperature (20-100ºC) and contact time (0-120 minutes) on the content of polyphenolic compounds and reducing sugars were the variables studied to ascertain the extraction optimum conditions. Statistical analysis evidenced that increasing the temperature has a positive effect only on the polyphenols extraction; meanwhile increasing the contact time has the same effect on the content of both reducing agents. Silver nanoparticles were obtained by putting into contact the above mentioned extract with silver nitrate solutions. Regarding this, the variables studied in this case were temperature, contact time, extract/metal solution volume ratio and pH. The instrumental analytical techniques used to follow the formation and the detection of silver nanoparticles were: UV/Vis, Field Emission Scanning Electron Microscopy (FE-SEM) coupled with Energy Dispersive X-ray (EDX) and Transmission Electron Microscopy (TEM). Results of these analyses showed: (i) a peak within the range 430-460 nm in the UV/Vis spectra that corresponds to the surface plasmon resonance of silver and indicates the presence of silver nanoparticles; (ii) most of the nanoparticles are present as aggregations as observed by electron microscopy characterization; (iii) EDX analysis confirmed the presence of silver on the observed nanoparticles.

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Notes

PP 18

Implementation of Fiber Optic Sensor (FOS) in Water Quality Monitoring

Boris Obrovski, Jovan Bajić; Ivana Mihajlović; Mirjana Vojinović Miloradov; Branislav Batinić; Miloš Živanov

Continual efforts have been made in the development of accurate and reliable new devices and equipment to provide modern monitoring program of different environmental media. The standard laboratory methods are generally accepted and reliable, however, they have certain limitations. Disadvantages are related to the use of expensive and specific chemicals, the complexity of the analysis, inability to obtain immediate results, and the loss of the analyte in the process of sampling, transportation, extraction and storage. Existing disadvantages of laboratory analyses demands new approach in developing of sensors for monitoring of water quality.

Fiber optic sensor (FOS) represents convenient method for monitoring of different aquatic media. FOS used in this research represents original color sensor which measure concentrations of six chemical parameters in different water bodies (surface water, groundwater, swimming pool). FOS converts RGB (Red-Green-Blue) color model to HSV (Hue-Saturation- Value) color model. S and V value were used for determination of analyte concentration. H parameter was used for the calculation of wavelength at which applied sensor measures the concentration of selected chemical parameters. Advantages of this color FOS are: simple to use, low-cost device, small dimensions, resistant to electromagnetic influences and corrosion and electric power is not required at sampling points.

Designed FOS is calibrated for measurement of residual and total chlorine, orthophosphate, nitrite, sulfate and hexavalent chromium in laboratory controlled conditions. Concentrations of chemical parameters in water samples were analyzed by original FOS method and results were compared with standard analytical EPA and HACH Methods with UV-VIS spectrophotometer (DR 5000, HACH, Germany). Measurements were carried out to confirm reliability, accuracy and reproducibility of results obtained with the FOS.

Relative differences in concentrations obtained with sensor and standard UV-VIS equipment ranged from 2.31 % for sulfate to 6.20 % for total chlorine. The results demonstrate the use of FOS as a laboratory “low-cost” device for measurement of selected chemical parameters in swimming pool water and surface water as a substitute for expensive standard analytical equipment. Future research should be aimed to develop in-situ mobile sensor for water quality monitoring.

The authors acknowledge for the funding provided by the Ministry of Education, Science and Technological Development of Republic of Serbia under project III43008.

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Notes

PP 19

Occurrence and Removal of Organic Pollutants in Municipal Wastewater Treatment Plants (WWTPs) of the Tropical City Haikou, China

Jan Schwarzbauer; Yuehua Huang; Larissa Dsikowitzky; Fei Yang

Strongly varying water flows in wastewater treatment plants (WWTPs) impede an efficient removal of organic contaminants. This is a huge challenge for wastewater management in particular in tropical areas with their strong seasonal rainfall patterns. Haikou is the most populous city of Hainan province, a tropical island located in the South China Sea. Hainan is the smallest and southernmost province of China. Typhoons regularly affect Hainan Island during the hot and wet summer monsoon season. The greater water-volume inputs to the two central WWTPs of Haikou during the periods of very heavy rainfall likely affects the removal of organic pollutants.

The aim of this study was a comprehensive characterization of the relevant organic pollutants in the cities' municipal wastewaters and, complementarily, an evaluation of the concentration levels before and after wastewater treatment during two seasons with different water flow regimes. The water samples were taken in 2015/16 shortly after a typhoon event and during the dry season in winter, respectively. Additionally, the urban coastal waters receiving the WWTP effluents were assessed.

Applying a non-target screening, around 60 relevant organic pollutants were identified in the wastewater samples. These contaminants include flame-retardants, synthetic fragrances and plasticizers that are all well-known household chemicals and have frequently been described from many world regions. In contrast, the spectrum of pharmaceutical drugs included compounds that were rarely reported as municipal wastewater constituents to date. The cough suppressants oxolamine and ansimar, the anaesthetic ketamine, the antifungal agent griseofulvine and the antibiotic dimetridazole were detected in the WWTP process water samples. Marmesin was also identified that occurs naturally in plants and was recently reported as a potential therapeutic agent for the treatment and prevention of angiogenesis-related diseases including cancer (Kim et al. 2015). Relevant biocides/pesticides were paclobutrazol, prometryn and atrazine. All biocides/pesticides were retrieved in the urban surface waters, whereas the pharmaceutical drugs except ketamine were not found. The contamination levels and removal efficiencies will be evaluated in detail.

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Notes

PP 20

Removal of Chlorinated Ethenes from Groundwater Using Iron-based Nanomaterials: Laboratory Analysis Results and Pilot Applications

Jana Oborná; Ondřej Lhotský; Ivo Medřík; Lucie Cádrová; Jana Steinová; Jan Filip

Chlorinated hydrocarbons are common environmental contaminants frequently found in groundwater and soils. These substances are dangerous due to their persistence, toxicity, potential carcinogenicity and the ability to accumulate in biological systems and food chain [1, 2]. Removal of these organic pollutants is an important challenge in the field of advanced water treatment. In recent years, materials containing nanoscale zero-valent iron (nZVI) particles have been increasingly used for abiotic reductive remediation methods. nZVI has excellent remediation characteristics such as high reactivity, good migration properties in the soil and, when combined with the carbon matrix, also sorption properties [3, 4]. Low toxicity of iron oxide, which forms after application of nZVI in anoxic conditions, is also an indisputable advantage of using nZVI [5].

This poster presents laboratory analysis results of groundwater (sampled from anonymous locality, Czech Republic) containing above-limit concentrations of vinyl chloride (VC), cis-1,2-dichloroethylene (DCE), trichlorethylene (TCE) and perchlorethylene (PCE) and their removal by iron nanoparticles (i.e. materials for reductive wastewater treatment technologies) and also by applying composite materials based on iron nanoparticles and carbon matrix (materials for reductive-sorption technology). Decrease of chlorinated ethenes was measured using HS-SPME-GC/MS technique. Iron nanoparticles were applied at concentration of 5 g/L for 14 days reducing the concentration of vinyl chloride, cis-1,2-dichlorethylene, trichlorethylene and perchlorethylene by 94.2, 58.4, 95.7 and 71.6 % respectively. Pyrophoric nZVI was selected for prospective pilot application based on laboratory test results. Following the pilot application of pyrophoric nZVI, the decline chlorinated ethenes will be monitored. qPCR methods are going to be used to monitor increase of iron reducing bacteria after the pilot application.

This work was supported by grant from the EU FP7 (project NANOREM) and Technology Agency of the Czech Republic "Competence Centers" (project No. TE01020218) and Research Infrastructure NanoEnviCz (LM2015073).

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Notes

PP 21

Polar Pesticides in Surface and Waste Water

Josef Caslavsky; Tereza Boruvkova

This study is focused on the determination of polar pesticides in surface and waste waters. In this study Mecoprop-P, MCPA, Dichlorprop-P, 2,4-D and MCPBA in differently loaded surface waters and communal waters from sewage treatment plants were analyzed. These herbicides are included in the group identified as environmental quality standards. Some of herbicides (2,4-D and MCPA) were selected because their consumption in the Czech Republic exceeds 30 tons per year. Samples were collected from three rivers in the Czech Republic near the town of Jaroměř (Elbe, Úpa and Metuje Rivers), from one river flowing through the town of Brno (Svratka River) and from inflow and outflow of two waste water treatment plants (WWTP Jaroměř, WWTP Brno – Modřice). Particular rivers were chosen for monitoring due to the probability of occurrence of herbicides, because they flow through agriculturally cultivated areas. Solid phase extraction (SPE) was used for the isolation of target compounds and their concentration. Gas chromatography with tandem mass spectrometry (GC/MS/MS) was used for the determination of target analytes in surface and waste waters after their derivatization.

Selected herbicides were detected in all collected samples. Their levels in surface waters were within the range of 0.1-100 ng/L, in waste water from 0.2 to 50 ng/L. The most contaminated was the water in the river Elbe. In common, the concentration of selected pesticides in outflow from the waste water treatment plants were lower than those in the recipients, in spite of the fact that removal efficiencies for these compounds were not very high (around 50 %, in some cases even worse).

Study was supported by the project No. FCH-S-16-3364 Environmental contamination by contaminants of inorganic and organic origin from the Ministry of Education, Youth and Sports of the Czech Republic.

Notes

PP 22

Just Go with the Flow: The Routine Application of GC×GC-TOF MS to Real-world Analyses

Laura McGregor; Matt Edwards; Nick Bukowski

Comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOF MS) has gained much popularity in recent years. The enhanced separation offered by the coupling of columns of complementary stationary phases has been proven to work well for a range of challenging samples; including petrochemicals, fragrances/food aromas and environmental contaminants. While GC×GC-TOF MS has been heavily adopted in research and development labs, it is rarely applied for routine analyses, with many analysts believing it to be too complicated, fragile and/or expensive. Furthermore, the thermal modulation devices which have dominated GC×GC literature require a cryogen fluid to modulate volatiles in the C4-C8 range – meaning additional running costs and the extra hassle associated with health and safety management of the laboratory.

This presentation explores the use of flow-modulation in routine applications, as a simple, yet effective, method of gaining all the benefits of GCxGC-TOF MS without incurring any of the historical cost or hassle.

Notes

PP 23

Assessment of the Degradation Pathway, Persistence and Eco-toxicological Impacts of Human Pharmaceuticals and Degradation Products in the Aquatic Environment

Lydia Niemi; Stuart Gibb; Zulin Zhang

Pharmaceutical compounds are extensively used in contemporary society, and once administered can be introduced into wastewater systems as either the parent drugs or in metabolised form. Inadequate wastewater treatment can result in these biologically active compounds being discharged into the aquatic environment via effluent from wastewater treatment plants. The effects of wastewater treatment on pharmaceutical removal are not fully understood and little work has been undertaken to characterise the removal, formation and fate of degradation products. Further research into the presence, persistence, degradation and eco-toxicological effects of these pollutants is therefore necessary to protect water quality and avoid eco-toxicological impacts in aquatic ecosystems.

This research aims to characterise pharmaceutical behaviour, degradation and fate during wastewater treatment and in receiving waters, and also to assess the eco-toxicity of select pharmaceuticals and degradation products. Various sampling and monitoring experiments of target compounds will be carried out, including degradation studies and toxicological tests with optimised analytical techniques such as LC-MS/MS, and novel chemical and bioassay methods such as E-SCREEN cell proliferation. It is anticipated that the effects of different treatment methods on pharmaceutical removal and degradation at separate stages of the treatment process (primary, secondary, tertiary) will also be investigated. The outcomes of this research will offer new insights into pharmaceutical behaviour during wastewater treatment and the subsequent effects in receiving waters, and also point to innovative and advanced solutions for increasing removal efficiencies, improving water quality and lessening the environmental risk of these compounds.

This research is funded by the Scottish Government Hydro Nation Scholars Programme in association with the Centre of Expertise for Waters (CREW).

Notes

PP 24

Teeth as a Proxy for Arsenic Exposure – A Study on Seaweed-Eating Sheep using HG-AFS and LA-ICP-MS

Magdalena Blanz; Kate Britton; Karen Grant; Eva Krupp; Jörg Feldmann

Assessing the extent of an individual's exposure to arsenic is a key aspect in the study of arsenic poisoning, which may occur due to e.g. proximity of ore-smelters, high arsenic levels in drinking water, or deliberate poisoning. In an archaeological context, investigation of arsenic exposure by analysing blood or urine is usually impossible, so that hair, bone and teeth are studied instead. However, due to the toxic effects of many arsenic species, there are few dedicated studies of how arsenic accumulates in these tissues.

This study investigates the accumulation of arsenic in teeth from modern-day North Ronaldsay sheep that were naturally exposed to high levels of arsenic (about 35 mg As per day, of which about 86 % bioavailable) by eating seaweed. Using HG-AFS, arsenic concentrations ranging from 0.3 ± 0.03 to 2.9 ± 0.2 mg/kg were measured in pooled dentine, cementum and pulp samples, which is over two orders of magnitude higher than in control populations. When comparing between individuals, a linear correlation was found with respect to the ratios of total arsenic content in second to third molars taken from the same individuals.

Using LA-ICP-MS, bioimaging of cross-sections of the sheep molars showed that arsenic predominantly accumulates in cementum, as well as in occlusal dentine (exposed dentine on the chewing surface). While the accumulation of arsenic in cementum may also originate from metabolic processes, increased arsenic concentration at the occlusal surface is thought to occur due to direct contact with arsenic during mastication.

MB is grateful for financial support from the European Social Fund and Scottish Funding Council as part of Developing Scotland's Workforce in the Scotland 2014-2020 European Structural and Investment Fund Programme.

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Notes

PP 25

Characterization by Fluorescence Spectroscopy (EEMs) and Parallel Analysis Factor of Humic like Substances Used as Additive in Photo-Fenton Processes

Margarita Mora Carbonell; M. Mora; S. García Ballesteros; P. Micó; R. Vicente;A. Arques; A.M. Amat

Since dissolved organic matter (DOM), concentration and chemical composition influences the intensity and shape of the fluorescence spectra, fluorescence excitation-emission matrix spectroscopy has been demonstrated as a sensitive technique to analyse it [1]. PARAFAC has demostrated its ability to decompose EEMs into independent varying fluorescent components [2]. Bio-Based Substances (BBS) obtained from urban water are able to expand the pH region of the photo-Fenton processes until near neutral pHs [3]; this effect seems to be ruled by the interaction between Fe(III) and BBS. This study set up to investigate the interaction of BBS with Fe(III), as well as the transformation of BBS in the photo-Fenton process at different pHs using fluorescence spectroscopy.

In this study Fluorescence excitation-emission matrix (EEM) spectroscopy was used to study the interaction between bio-base substances (BBS) obtained from urban waste and Fe(III) and the transformation of BBS when used as additive in photo-Fenton processes. Parallel factor analysis (PARAFAC) was used to characterize the EEM dataset from BBS, BBS-Fe(III) mixtures and BBS degradation at three different pHs. Three different components were obtained in all cases.

The financial support of the European Commission H2020-MSCA-RISE-2014 (Project number: 645551), the Spanish Government (CTQ2015-69832-C4-4-R) and the Generalitat Valenciana (GV/2015/074), and Predoctoral fellowship for S. García.

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Notes

PP 26

Hydrous Manganese Oxide (HMO) Process in Potable Water Treatment for Radium, Iron and Manganese Removal

Marika Viisimaa; Nele Nilb; Madis Kiisk; Siiri Suursoo; Anna Goi

According to the Estonian Regulatory Act (RTL 2001/100/1369, 2015) the concentrations of iron, manganese and radium isotopes (^{226}Ra and ^{228}Ra) in the groundwater of Estonia from Cambrian-Vendian and Ordovician-Cambrian aquifers exceed the potable water threshold limits. The Hydrous Manganese Oxides (HMO) process is known as innovative treatment method that allows removing iron, manganese and radionuclides in water. The HMO reagent is referred as the mixture of the potassium permanganate ($KMnO_4$) and manganese sulfate ($MnSO_4$) combined aqueous solution.

The pre-treated by aeration water without pH pre-adjustment (pH 8.1) contained 0.23 mg Fe/L, 0.14 mg Mn/L and 0.45 Bq/L of 228Ra activity concentration. While the iron after the aeration was possible to remove completely by the following filtration, the concentration of manganese remained without a change indicating to its soluble state. This did not satisfy the potable water threshold limit of 0.05 mg manganese per L set by the Estonian Regulatory Act (RTL 2001/100/1369, 2015). Some decrease in the 228Ra activity concentration was observed; however, it was not enough to achieve the set radiological parametric value for indicative dose of 0.1 mSv/y. Thus, the efficacy of the HMO process for pre-aerated groundwater purification from the excess of manganese and radium in columns was evaluated.

The results of the experiments showed that manganese removal in the pre-treated by aeration water improved with the HMO dosage increase. A two-fold upsurge of HMO dosage from 0.5 to 1.0 mg per L of the treated water resulted in the residual manganese concentrations of 0.05 and 0.02 mg/L, respectively. Complete removal of iron and high removal of radium (up to 80%) were achieved at all the HMO dosages (0.5, 0.75 and 1 mg per L) applied. The addition of the moderate HMO reagent dosages (0.5-1.0 mg per L) without the reagent pH regulation did not change the pH of the treated water. The particulates formed during oxidation of iron and manganese by aeration and the HMO reagent, as well as, excess $KMnO_4$ were subsequently removed by filtration through a 0.45µm membrane filter.

The combination of aeration and the HMO process applied for the groundwater treatment allowed satisfying the threshold limits set for the drinking water and can be implemented as effective treatment technology for iron, manganese and radium removal in the groundwater potabilization.

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Notes

PP 27

Removing Organic Contamination from Water Using UV Radiation

Martina Repková; Petra Venská

Pyridine and pyridine derivatives (PPDs) represent an important group of environmental pollutants widely used as industrial solvents for production of pesticides, dyes, pharmaceuticals etc. or as production intermediates. These compounds naturally occure in the environment but the excessive use in industry and agriculture leads to higher concentrations in surface and ground water. Presence of PPDs in the environment is a potential risk for ecosystems and human health, such as liver damage, harmful effects on immune system and reproduction. Industrial waste water with higher levels of PPDs are toxic for water ecosystems and cause undesirable odour and taste. There is a need to remove PDDs from waste water and many different options for treatment have been developed including physical (for example adsorption on different material of ultrafiltration), chemical (based on use of chemical or photochemical oxidation, coagulation) and biological methods (large scale of different microorganisms). The thesis focuses on using UV radiation to degrade pyridine and some pyridine derivatives under different conditions. Photolysis of pyridine produces various organic products. Most likely the carboxylic acids are formed while the ring is opened and NH^{4+} and formamide are released. Small amount of pyridine is transformed to 2-hydroxyl pyridine. On the other hand, the degradation of 2-halogened pyridines leads mostly to formation of 2-hydroxyl pyridine. Few pathways of this degradation were proposed in which pyridine absorbs photons or is attacked by free radicals. Several methods to determinate pyridine in different types of matrix have been reported – for example HPLC, GS, GS-MS or spectrometry. Succinic acid – as the main product of degradation – is possible to be determinated by chromatographic methods.

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Notes

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Application of $\delta^{13}C$ and $\delta^{15}N$ as Isotopic Proxies in Organic Geochemical Study of Lignite

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The study aims to explain the usage of isotopic proxies in determining the sources of organic matter (OM), post-depositional alteration processes (such as thermal alteration) and primary productivity (Hollander and McKenzie, 1991). The isotopic analysis was done to evaluate the contributions of these factors to the observed isotope excursion on the samples from the deepest, coal seam III (83.65 – 123.00 m) of lignite from the Smederevsko Pomoravlje field, Kostolac Basin, Serbia.

The $\delta^{13}C$ values in examined lignite samples range between -27.09 to -25.95 ‰ (average, -26.31 ‰) which is in accordance with the results of carbon isotopes in other coals worldwide (Holmes et al., 1981). These results and their correlations with total organic carbon (TOC) and C29 sterene contents suggest peat formation from terrigenous background and that maturity had no influence on the organic carbon isotope composition of analyzed coal. The $\delta^{15}N$ values of investigated samples have a range between 2.89 ‰ and 4.52 ‰ and mean value of 3.43 ‰. Nitrogen isotope proxy can be used to distinguish between marine and terrestrial OM, with marine OM being isotopically heavier due to fractionation during nutrient uptake and terrestrial OM being relatively lighter since fractionation here is low or even absent (e.g. Wada et al., 1987). Williams et al. (1995) suggested that ammonia has been produced by irreversible reactions without any isotopic fractionation. Also previous studies demonstrated that molecular nitrogen derived from OM has a low $\delta^{15}N$. For studied samples it would be possible that molecular nitrogen was not an important primary product of the lignite denitrogenation.

In this case, carbon and nitrogen isotope data of coal indicate their derivation from the terrestrial source, which is in accordance with the results of other geochemical and petrological parameters applied on these samples. Different values of $\delta^{13}C$ and $\delta^{15}N$ could be related to different lythotypes of the samples. The maximum values were observed for mixture of xylite-rich and matrix coal and minimum values for xylite-rich lithotype. Explained proxies can be successfully used to complement the image in biogeochemical investigation of lignite.

The study was financed by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project number 176006) and the Swedish Foundation for International Cooperation in Research and Higher Education (STINT).

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Semi-volatile Organic Contaminants Trapped in Environmental Matrices – Methods to Release Them

Nuno Ratola; Vera Homem; José Avelino Silva; Sara Ramos; Lúcia Santos; Arminda Alves

The number of contaminants being released into our environment is endless and obviously pose a multitude of challenges to research scientists. A myriad of different properties and characteristics have an effect on their life cycles, behaviour and patterns. Moreover, all the matrices serving as transport media or sinks for these pollutants hold precious information on the levels of some chemicals, but keep these data trapped in a way that requires sometimes complicated analytical set-ups that need to be constantly improved, in order to obtain better compound resolution and lower limits of detection, keeping the budget and the environmental impact as small as possible. In fact, the extraction and analysis of environmental matrices (such as vegetation, soil, air, among others) require effective extraction and clean-up procedures to retain the target compounds and eliminate lipid material and other kinds of interfering elements. The development of multi-matrix studies, still scarce in literature (Silva et al., 2015), is an important short-cut to come up with expedite protocols that allow a comprehensive assessment of the presence of numerous contaminants.

In this presentation we review the different protocols our group has developed in the recent years to “release” and quantify the levels of semi-volatile organic contaminants (SVOCs) in diverse sampling media. More classical procedures based on Soxhlet or ultrasonic extraction and clean-up phases like solid-phase extraction (SPE) or gel permeation chromatography (GPC) were employed before quantification by GC-MS, but also new more environmentally approaches such as ‘Quick, Easy, Cheap, Effective, Rugged and Safe’ (QuEChERS) technique (Prestes et al., 2011) will also be reported. Legacy and emerging compounds were the targets of our studies: brominated flame retardants (BFRs), polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), polycyclic aromatic hydrocarbons (PAHs) as the former and synthetic fragrances (musks) and volatile methyl siloxanes (VMSs) as the latter.

Methods are presented in terms of validation parameters (detection limits, recovery) and some results from field sampling studies. The quantification was always performed using internal standards, mainly deuterated compounds.

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Notes

PP 30

Treatment and Reuse of Textile Effluents by Mild Sonar Photo-Fenton in the Presence of urban Waste Extracts

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The possibility of reuse the effluents generated by finishing textile industries for new dyeing baths, represents a major advanced against serious environmental problem that generates this type of industry characterized by high water consumption, an elevated content of complex organic matter, conductivity and intense colour (Ghaly et al. 2014).

The advanced oxidation processes (AOPs) seems a meaningful alternative for the treatment and reuse of textile effluents. AOPs include a group a treatments that are based on the generation of highly oxidizing species as hydroxyl radical and that are able to remove recalcitrant pollutants and they have been applied on these effluents (Rosa et al. 2015). Solar photo-Fenton is an AOP that is based on the ability of iron salts to decompose hydrogen peroxide into reactive species, mainly hydroxyl radical (Pignatello et al, 2006), with the difficulty that it needs a very acidic pH, close to 3, for proper operation. To overcome this problem, complexing agents are being used to extend the applicability of photo-Fenton towards milder pH (Huang et al. 2013).

The presence of extracts from urban waste (BOS), obtained from a mechanical-biological treatment of wastewater (Montoneri et al. 2008), has permitted to use a solar photo-Fenton treatment in conditions closer to neutrality (pH 5), to remove the colour of these textile effluents and to reuse in subsequent dyeing processes of cotton with direct dyes, thus reducing the consumption of water. Laboratory scale experiments carried out with synthetic effluents and real effluents shows that comparable results were obtained when using as solvent water treated by photo-Fenton with SBO and fresh deionized water in dyeing processes.

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PP 31

Adaptation of Screening Analysis Method for Meat Industry Wastewater Sample

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The negative impact of untreated industrial wastewater on water bodies is one of the main environmental issues. Since the meat industry effluent discharge may cause alarming contamination of surface and ground water [1], the research was focused on the adaptation of screening analysis method for the sample of meat industry wastewater. The GC-MS technique was selected as a conventional method for screening analysis of organic compounds in complex environmental matrices. Several sample preparation methods have been tested while different solvents have been used during the liquid-liquid extraction to obtain the optimal method for the analysis. An optimal solvent should have a broad range of properties that enable extraction of the highest percentile of metabolites in the highest possible yields, with good reproducibility [2], without affecting the stability of the extract [3]. During the study, three different solvents (n-pentane, DCM and methanol) were used to determine the most adequate for the selected sample type. The extraction into DCM favours the transport of hydrophobic organic compounds [4]. The evaporation was conducted on Kuderna Danish apparatus. The evaporation procedure in methanol lasted for approximately 6 hours, depending on a room temperature, and it was disregarded within the evaluation of obtained experimental data. Using GC-MS analysis, 1,125 peaks were detected in samples prepared with the n-pentane and DCM and 313 substances have shown quality match index (QMI) greater than 65%. DCM had higher quality extraction with significantly less pick deterioration and distortion. Maximum number of peaks was detected using the DCM. Average difference in pick acquisition was 38.34% in favour of sample prepared with DCM. Identification percentage for both solvents was in the range of 62% to 67 %, slightly higher in favour of n-pentane. The optimal procedure for the preparation of the meat industry samples prooved to be LLE with DCM as solvent, coupled with Kuderna Danish apparatus for the sample concentration.

The research is supported by the Ministry of ESTD, RS (III 46009).

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Notes

PP 32

The Importance of POPs Contamination Monitoring Programmes on Landfill Sites in Serbia

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During the past decades, pollution by organic substances that are used daily, or that are formed as by-products of industrial production processes, focuses the research on the detection and quantification of persistent organic pollutants (POPs) in various environmental media. In past years special attention is addressed on the pollution from landfill sites because of the bad waste management practice. Inadequate waste treatment is one of the most serious environmental problems in Serbia (Batinic et al., 2011). The big lack in Serbia is low involvement of stakeholders which is very important for achieving sustainable municipal solid waste management practice.

The pollution caused by non-controlled and/or semi controlled landfilling is even worse by the fact that many landfills are still operating without an appropriate impermeable bottom liner and an effective collection and treatment systems (Lema et al., 1988). Serbia as a developing country with GDP of 0, 8% (2015) and poor waste management practice is significantly vulnerable regarding the impact that landfills have on the surrounding environment. There are about 3500 identified landfills in Serbia, of which 165 are municipality landfills, 5 are sanitary landfills and rest are open dumps. Also there are 5 regional sanitary landfills in construction progress. The National legislative prescribe the time frame for the monitoring of generated leachate during active and passive phase of landfill but does not highlight the parameters that should be monitored in leachates as well as the permitted values and does not include other environmental media such as ambient air and soil.

The investigation on landfilling process as a possible source of POPs has never been conducted before in Serbia. The contamination pathways of POPs from landfills depend on their specific physicochemical properties, water solubility and volatility and the characteristics of landfill environment. Previous study (Preliminary qualitative and quantitative analysis of leachate water and gas from the waste landfills for establishment of continuous monitoring, 2008-2009) has shown that leachate samples collected on selected landfill sites in Serbia include compounds which can be hazardous to human health and the environment but did not include information on POPs levels. The presence of hazardous compounds in landfill leachates, many of which have not yet been identified, could have a significant impact on landfill risk assessments as well as on human health and environment pollution.

It can be concluded that further investigations should consider determination of POPs concentration levels dependence of the structure of municipal waste landfill as well as determination of temporal concentration trends and distribution pathways of POPs in the air phase / soil / water on landfill sites.

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Notes

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Activated Carbon from *Prunus Armeniaca* Biomass: Optimization of Heavy Metal Removal

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Heavy metal pollution of aqueous media and industrial effluents is one of the most significant environmental problems. Heavy metal contamination exists in aqueous waste streams of many industries in Serbia, such as mining operations, surface finishing industry, paper or pulp industries and energy or fuel production. Heavy metals are toxic and non-biodegradable pollutants that may cause a variety of diseases and disorders when they accumulate in living tissues [1]. Several methods have been reported for the removal of these pollutants from wastewaters, including chemical precipitation, ion exchange and adsorption. Among these methods, adsorption on low-cost activated carbon obtained from industrial waste byproducts is one of the most effective, economic and simplest methods [2].

In this work, apricot stones (*Prunus armeniaca* biomass) was used as a precursor for the preparation of activated carbons by phosphoric acid activation. The effects of pH, adsorbent dosage, contact time and initial concentration of Pb^{2+}, Cd^{2+} and Ni^{2+} on the adsorption were studied in a batch process mode. Industrial effluents are mainly contaminated with more than one heavy metal. In order to assess the multicomponent effects on separation efficiency, adsorption in binary and ternary metal systems was investigated. Diluted phosphoric acid obtained after the filtration process within preparation of adsorbent was chosen as the desorbing agent.

Produced activated carbon shows promising adsorption capacity for metal ions removal. A dose of 2 g L^{-1} of adsorbents in solutions with an initial pH of 6.0, an initial adsorbate concentration of 100 mg L^{-1} and a contact time of 30 min resulted in the maximum metal ions removal efficiency. The Freundlich isotherm gave a better fit than the Langmuir isotherm revealed that the adsorption was potentially multilayer. The monolayer adsorption capacities, qmax, calculated from Langmuir model were 172.4, 112.7 and 63.7 mg g^{-1} for the Pb^{2+}, Cd^{2+} and Ni^{2+}, respectively. Further, the adsorption kinetics followed a Lagergren pseudo second-order model, which implied that the adsorption was mainly a chemisorption process. Results indicated that the separation efficiency of single metal ions in all multisolute systems decreases with the increasing number of components with the preferential affinity of metal ions in following order: $Pb^{2+} > Cd^{2+} > Ni^{2+}$. Based on desorption study results, activated carbon was successfully regenerated with diluted phosphoric acid for 3 cycles.

It may be concluded from the above presented results that activated carbon from apricot stones (*Prunus armeniaca* biomass) can be considered as a potential adsorbent used for the elimination of metal ions from wastewater since it is a low-cost and locally available adsorbent.

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PP 34

Hydrodeoxygenation of Guaiacol: A Model Reaction for the Upgrading of Lignin-derived Biooils

Simone Ansaloni; Nunzio Russo; Raffaele Pirone

The exploitation of lignocellulosic resources for the production of fuels and chemical has attracted increasing attention in the last decades. The lignin fraction is underutilized despite the enormous potential as source of renewable aromatic compounds[1]. To support the development of modern biorefineries new catalityc processes are needed in order to effectively transform the ligno-derivates into useful building blocks. Guaiacol is one of the main compounds present in bio-oils derived from the cleavage of the lignin structure, in this sense, we studied the hydrodeoxygenation (HDO) of guaiacol as a model process for the upgrading of lignin-derived bio-oils[2]. Reactions were carried out in a batch reactor at 350°C and 40 bar of H_2 for 1h residence time, in the presence of dodecane as solvent and several Mo-based catalysts prepared by impregnation of ammonium molybdate on various supports (SiO_2, Al_2O_3, NaY zeolite, MgO, active carbon, graphite). Different catalytic behavior was shown due to diverse surface area, acidity and active phase. Mo on active carbon (Mo/C) showed the best performances towards guaiacol demethoxylation with 72% of selectivity to phenol and 19% to p- and o-cresol. Active carbon results to be the best support due to the high surface area and low acidy, while it allows great dispersion of MoOx which exhibits characteristic fragments with lamellar shape, capable to provide large active surface with localized acidity. Moreover, the effect of temperature, H_2 load, residence time and metal percentage on the HDO performances were investigated over Mo/C.

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Understanding the Fate of Active Pharmaceutical Compounds in Surface Waters Receiving Poorly or Untreated Sewage Effluent and the Development of Appropriate Environmental Risk Assessment Approaches

Simone Bagnis; Mark Fitzsimons; Jason Snape; Alan Tappin; Sean Comber

Active pharmaceutical compounds (API's) have been classified as emerging contaminants, and their introduction in the environment might pose risks to ecosystems. The main source of pharmaceuticals in the environment is human use and excretion or the improper of unused mediation to the sewerage system. In wastewater treatment works the lack of efficient removal of some pharmaceuticals, combined with pseudo-persistence, results in their presence in surface waters. As patient access to medicines increases in developing countries the environmental concentration of pharmaceuticals has the potential to be higher than in developed countries if the level of wastewater and drinking water treatment does not also increase.

Untreated wastewater enters the environment via discharge into surface waters resulting in a downstream area characterized by high pollution, named "impact zone". Characterization of the environmental risk posed by pharmaceuticals in such an area is challenging since the formal protocol for environmental risk assessment was developed for environmental conditions largely different from the ones encountered in the impact zone; High levels of BOD, ammonia, and other potential toxicants exist in combination with low concentrations of dissolved oxygen, meaning that there is an absence of traditional species used for toxicological endpoints. Therefore, the calculation of predicted environmental concentrations (PEC) in such conditions is not relevant.

The aim of the research is to obtain a comprehensive overview of the gaps regarding the fate of pharmaceuticals in aquatic environment initially starting with an extensive literature review of available data for (1) occurrence, (2) degradation rates, (3) partitioning to dissolved organic matter, colloids and suspended solid matter, and (4) relevant endpoints. This will inform experimental research aimed at gaining data about partitioning and degradation of selected pharmaceuticals in the impact zone at varying dilutions, and determination of proper endpoints.

The information obtained will be used to develop an environmental risk assessment approach for impact zones, as only with more accurate exposure concentrations and impact data can the risks to the aquatic environment of APIs be quantified.

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PP 36

Review on Phytoremediation of Heavy Metal Contaminated Soil: A Case Study in Hunan Province, China

Stuart Gibb; Xie Min; Xu Yao, Julong Sun, Xiaobo Liu, Xiong Ren

Compared with the traditional environmental remediation technology, the plant soil remediation has the advantages of low cost of governance, compatibility of environmental aesthetics, and in situ treatment process. Present status of heavy metal pollution in soil and several types of phytoremediation are reviewed in this paper, mainly encompasses phytoextraction, phytovolatilization, hyperaccumulator, along with the advantages and disadvantages of phytoremediation. The sources of heavy metal pollution in Hunan Province China were emphasized and the development direction and prospect of phytoremediation in contaminated soil concerning the principle, examples, and the advantages and disadvantages were stated in order to provide the guidance for the sustainable management and research heavy metal remediation in soil.

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Notes

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Comparison of Methods for Analysis of Chlorinated Phenols in Water

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Three methods for analysis of chlorinated phenols in water were compared: liquid – liquid extraction (LLE) after derivatization; solid phase extraction (SPE) after derivatization; and stir bar sorptive extraction (SBSE) with in situ derivatization, followed by liquid desorption. First two methods were conducted according to the analytical procedure developed by (Soniassy et al., 1994), while the third method was modified after (Paasivirta et al., 1990).

The chlorophenols used in this research were: 2,4 – dichlorophenol, 2,4,6 – trichlorophenol, 2,3,4,6 – tetrachlorophenol and pentachlorophenol. Water samples were prepared using distilled water spiked with the chlorinated phenols standard solution, so that the absolute content of phenols in water was in the 50 ng/L to 500 ng/L range. Additionally, water samples were spiked with the brominated phenols surrogate standards: 2,4-dibromophenol and 2,4,6-tribromophenol. Chlorophenols and bromophenos were derivatized to acyl derivatives directly in the water samples with acetic anhydride, under basic conditions. For LLE dichloromethane was used as a solvent to extract the investigated compounds. For SPE, the investigated compounds were concentrated on C18 solid phase extraction cartridges, and extracted with methanol. SBSE was conducted using Twister stir bar with PDMS stationary phase. The analytes preconcentrated on the stir bar were desorbed in an ultrasonic bath using ethylacetate as a solvent. The extracts were analyzed by GC-MS in selected ion monitoring mode.

The method comparison study included analysis of linearity, limit of detection (LOD), limit of quantification (LOQ), and sensitivity for all methods used. All methods were shown to be linear in the investigated range of concentrations. However, LLE demonstrated the highest sensitivity, the lowest limit of detection and the lowest limit of quantification, and, accordingly, is a method of choice for analyses of investigated group of chlorophenols in water samples.

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Analysis of Dibenzothiophene Biodegradation Products During ex situ Bioremediation of Soil Contaminated with Oil Pollutant

Tatjana Šolević Knudsen; Jelena Milic, Mila Ilić,; Srđan Miletić; Vladimir Beškoski, Gordana Gojgić-Cvijović, Miroslav M. Vrvić

The aim of this work was to investigate dibenzothiophene (DBT) biodegradation products formed during ex situ stimulated bioremediation of a soil contaminated with heavy residual fuel oil. A detailed description of the contaminated soil used, bioremediation experiment and microbial community employed is given in our previous paper (Beškoski et al., 2011). Presence of DBT and its methylated homologues in this soil has already been confirmed, as well as microbial activity in biodegradation of these compounds (Šolević Knudsen et al., 2015).

During six-month long ex situ bioremediation experiment, soil samples were taken five times in regular intervals. The soil samples were extracted in a Soxhlet apparatus with dichloromethane as a solvent. The extracts were cleaned up and fractionated using column chromatography. Target compounds were analysed by gas chromatography – mass spectrometry (GC-MS). The GC-MS analysis comprised numerous DBT oxygenated and hydroxylated derivatives, which are known as intermediary products of different DBT biodegradation pathways (Monot and Warzywoda, 2008). Of all DBT derivatives investigated in this research, 2-hydroxybiphenyl (HBP) was the only one identified in the soil samples analyzed. HBP was identified in the soil samples in the final phases of the experiment, when DBT was present in a low abundance, and later, when DBT was almost completely degraded. Detection of HBP, which is a product of, and marker for the 4S DBT biodegradation pathway indicates that corresponding metabolism might also be operational in the microbial community employed in this research. Additionally, presence of HBP in the soil samples when DBT was almost completely degraded indicates that this compound might be useful indicator of former DBT presence in soil even when DBT is completely degraded. Finally, these results indicate that biodesulfurization processes, which have already found application in removal of sulfur-containing compounds from crude oil and its derivatives, aiming at improving their quality, might also play a significant role in reduction of the environmental pollution from the fossil fuel contamination.

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Notes

PP 39

Analysis of *Cedrus Atlantica* (Atlas cedar) Needles as Potential Passive Samplers of Polycyclic Aromatic Hydrocarbons (PAHs) in Air

Tatjana Šolević Knudsen, Jelena Milić, Nenad Zarić, Ivan Gržetić

Cedrus atlantica (Atlas cedar) is an evergreen conifer that is common in cultivation as an ornamental tree in temperate climates. This decorative tree is very widespread in green areas in Belgrade, the capital of Serbia. Considering the fact that needles of some coniferous tree species are capable of accumulating, in their cuticular wax layers, semi-volatile and low-volatile organic compounds from the air (Ratola et al. 2011), this study was carried out to determine whether or not *Cedrus atlantica* pine needles can accumulate atmospheric PAHs, and, therefore, if they can be used as passive samplers of these compounds.

The needles of *Cedrus atlantica*, different in age, were collected in May 2016 in a city park in the city center of Belgrade. Presence of different PAHs in the air of Belgrade had already been confirmed by previous studies (Cvetković et al. 2015). In order to avoid possible erroneous conclusions that might be introduced by the sample preparation method, the samples were extracted using three different methods: ultrasonic extraction (Ratola et al. 2006), Soxhlet extraction (Ratola et al. 2006) and alkaline digestion followed by liquid-liquid extraction (Kelly et al. 2000). The extracts obtained by different methods were cleaned up and fractionated using column chromatography (Novaković et al. 2012). All fractions isolated were analysed by gas chromatography – mass spectrometry (GC-MS). The GC-MS analyses were focused on determination of presence or absence of the following compounds: naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benzo[a]anthracene, chrysene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[j]fluoranthene, benzo[e]pyrene and benzo[a]pyrene, indeno[1,2,3-c,d]pyrene, benzo[g,h,i]perylene, dibenzo[a,h]anthracene. Additionally, methylated homologues of 2 – 4 ring PAHs were analysed in the same way.

The different sample preparation methods gave very similar results. Presence of 3 and 4 ring PAHs was confirmed in the extracts of the pine needles investigated. Moreover, presence of mono- and di-methyl homologues of 3 and 4 ring PAHs in these extracts was indicated as well. The results of this research demonstrated that *Cedrus atlantica* pine needles are capable of accumulating 3 and 4 ring PAHs and their mono- and di-methyl homologues. Accordingly, it can be concluded that needles of this coniferous tree can be considered as passive samplers of these PAHs in the air.

[1] Cvetković et al., (2015) Concentration and source identification of polycyclic aromatic hydrocarbons in the metropolitan area of Belgrade, Serbia. Atmospheric Environment 112, 335-343; [2] Kelly C.A., Law R.J., Emerson H.S. (2000) Methods for analysis for hydrocarbons (PAH) in marine samples. Aquatic environment protection analytical methods Number 12; [3] Novaković et al., (2012) Degradation of methyl-phenanthrene isomers during bioremediation of soil contaminated by residual fuel oil. Environmental Chemistry Letters 10, 287–294; [4] Ratola N., Lacorte S., Alves A., Barcelo D. (2006) Analysis of polycyclic aromatic hydrocarbons in pine needles by gas chromatography–mass spectrometry–comparison of different extraction and clean–up procedures. Journal of Chromatography A 1114, 198–204; [5] Ratola N., Amigo J.M., Oliveira M.S.N., Araújo R., Silva J.A., Alves A. (2011) Differences between *Pinus pinea* and *Pinus pinaster* as bioindicators of polycyclic aromatic hydrocarbons. Environmental and Experimental Botany 72, 339–347.

Notes

PP 40

Source Apportionment of Polycyclic Aromatic Hydrocarbons in Street Dust of Belgrade, Serbia

Tatjana Šolević Knudsen; Tamara Đorđević, Nenad Zarić

The objective of this research was to investigate the origin of polycyclic aromatic hydrocarbons (PAHs) in the street dust of Belgrade, the capitol of Serbia. Additionally, the values of different PAH diagnostic ratios in different particle size fractions were compared as well. The street dust samples were collected in summer 2016 at three different locations. The samples were fractioned into three sizes with diameters of: The results showed that the PAHs in the samples investigated represent a complex mixture originating from different pyrogenic and petrogenic sources. The analysis of PAH diagnostic ratios in different particle size fractions demonstrated some differences. These differences were the lowest for low-molecular weight PAHs and the highest for the high-molecular weight PAHs.

Notes

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Particle-Size Distribution of Individual Polycyclic Aromatic Hydrocarbons in Street Dust of Belgrade, Serbia

Nenad Zarić; Tamara Đorđević, Tatjana Šolević Knudsen

The aim of this study was to investigate the differences in distribution of individual Polycyclic Aromatic Hydrocarbons (PAHs) in different size-fractions of particles in street dust of Belgrade, the capitol of Serbia. The street dust samples were collected in summer 2016 at three different locations. Using a set of stainless steel sieves the particles were fractioned into three sizes with diameters of: The results showed different distribution patterns of individual PAHs in different size fractions at different location. Additionally, at one sampling location, different grain size gradient was observed for low- and high-molecular weight PAHs. Accordingly, it can be concluded that distribution of individual PAHs in different street dust size fractions is influenced by size of the particles and size of the PAH molecules. However, it seems that the most significant influence on these distribution patterns are dust characteristics related to the sampling location.

Notes

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Origin of Polycyclic Aromatic Hydrocarbons in the City Park Soil, Tivat, Montenegro

Tatjana Šolević Knudsen, Blažo Lalević, Nikola Antić, Vera Raičević

The objective of this research was a source apportionment of polycyclic aromatic hydrocarbons (PAHs) in the city park soil in Tivat, Montenegro. Previous research of the soil from this area indicated high amounts of some heavy metals, PAHs, polychlorinated biphenyls and organotin compounds (Karlicic et al, 2014). The focus of our present research is identification of sources of PAHs identified in the samples from this locality. The composite soil sample from the city park in Tivat was extracted in a Soxhlet apparatus with dichloromethane as a solvent. The extract was cleaned up and fractionated using column chromatography. In the fraction of aromatic hydrocarbons, PAHs were analysed by gas chromatography – mass spectrometry (GC-MS) in a selected ion monitoring (SIM) mode. The ions monitored were: m/z = 128 (naphthalene), m/z = 152 (acenaphthylene), m/z = 154 (acenaphthene), m/z = 166 (fluorene), m/z = 178 (phenanthrene and anthracene), m/z = 202 (fluoranthene and pyrene), m/z = 228 (benzo[a]anthracene and chrysene), m/z = 252 (benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[j]fluoranthene, benzo[e]pyrene and benzo[a]pyrene), m/z = 276 (indeno[1,2,3-c,d]pyrene and benzo[g,h,i]perylene), and m/z = 278 (dibenzo[a,h]anthracene). Thereafter numerous PAH diagnostic ratios were calculated and analyzed. The PAH profile of the investigated soil sample was dominated by 4-, and 5-ring PAHs. Additionally, peaks originating from 6-ring PAHs were also prominent. The results indicated that non-traffic emissions were the principal sources of these PAHs and that they were mainly of combustion origin. However, some contribution from traffic was indicated as well. The results demonstrated that the principal combustion emission sources of the PAHs in the city park soil in Tivat were grass and wood combustion while the principal traffic source was from diesel engines.

[1] Karlicic et al., In situ Bioremediation of Soil Polluted with Organotin Substances. In: International Conference: Soil 2014: In: Vrvić, M., Cokić, Z., Tanasijević, Lj. (Ed.), Proceedings of the „Soil 2014“ Planning and land use and landfills in terms of sustainable development and new remediation technologies. Zrenjanin , Serbia, pp. 43-50.

Notes

PP 43

Bioremediation of Complex Contaminant from Petroleum Industry in an Artificial Soil Substrate

Tatjana Šolević Knudsen; Jelena Avdalović, Srđan Miletić; Mila Ilić, Jelena Milić, Vladimir Beškoski, Miroslav M. Vrvić

The objective of this research was to investigate the efficiency of bioremediation of complex contaminant from petroleum industry in an artificial soil substrate. The artificial soil substrate was prepared as a mixture of sand and sawdust. A complex contaminant from petroleum industry was added to make the final mass of the experimental biopile of 45 kg. During the experiment, the biopile was inoculated with multiplied consortia of microorganisms, isolated from the complex contaminant. Reinoculation was carried out every thirty days. The pile was mixed once per month to achieve the effect of aeration. Compounds of nitrogen, phosphorus and potassium were used for biostimulation. The results of this experiment were compared with the results of analyses of a control pile, which was prepared in the same way as the biopile but without inoculation, aeration and biostimulation. The experiment lasted 110 days.

Total Petroleum Hydrocarbons (TPH, as per method ISO/TR 11046:1994) in the biopile and the control pile were analyzed at the beginning, after 60 days, and at the end of the experiment. Total decrease of TPH in the control pile at the end of the experiment was 5.56 %. The analysis of the biopile showed a total decrease in TPH of 54.75 %. In order to investigate changes in distribution and abundances of different compounds during this experiment, TPH extracts from the biopile were analyzed by gas chromatography – mass spectrometry (GC-MS). The GC-MS analysis of TPH extract from the biopile at the beginning of the experiment showed that dominant compounds in this contaminant were isoprenoids and petroleum polycyclic aromatic hydrocarbons (PPAH): naphthalene, phenanthrene, dibenzotiophene and pyrene, and their C1-C4 alkylated homologues.

At the end of the experiment, most of the PPAH were reduced in abundances, and some of them were completely removed. The results of this research showed that bioremediation of petroleum pollutant dispersed in the artificial soil substrate can remove as much as 55 % of total petroleum hydrocarbons in 110 days. Considering the fact that the only compounds affected in this research were PPAH, it can be concluded that the procedure described can remove up to 55 % of PPAH from petroleum pollutant in relatively short period, which makes it especially attractive in environmental applications.

[1] Avdalović Jelena, Doctoral Dissertation, Generating of soil in the process of bioremediation, Faculty of Chemistry, Belgrade, 2015 (in Serbian); [2] ISO/TR 11046:1994 International standard: soil quality - Determination of mineral oil content - Method by infrared spectrometry and gas chromatographic method.

Notes

PP 44

Real time Monitoring of Sea Contaminants by an Autonomous Lab-on-a-chip Biosensor (SEA-on-a-CHIP)

Yann Aminot; James W. Readman; the Sea-on-a-Chip project consortium

Early warning systems that can provide extreme sensitivity with appropriate selectivity are required to assess chemical contamination of estuarine and coastal areas. An EU project SEA-on-a-CHIP (2013-2017) aims to develop a miniaturized, autonomous, remote and flexible immuno-sensor based platform in a lab-on-a-chip configuration combined with electrochemical detection for real time measurement of organic micropollutants in marine waters. This system is being developed for direct application in aquaculture facilities for the rapid assessment of 7 selected contaminants from 5 groups of compounds that affect aquaculture production (compounds which are toxic, bioaccumulative, endocrine disruptors) and also those produced by this industry that affect the environment and human health (antibiotics and pesticides). The seven selected contaminants for the 3rd prototype are irgarol, sulfapyridine, domoic acid, chloramphenicol, estradiol, PBDE 47 and deltamethrin. Plymouth University involvement in the project is mainly on the verification and validation of the performance of the immunosensors through conventional analytical chemistry.

This poster presentation explains how the sensors are validated in laboratory studies, under artificial mesocosms and during field experiments in aquaculture facilities. This includes the evaluation of potential interferences and the applicability of the sensors to broader environmental assessments of contamination. Further information on this project is available at: www.sea-on-a-chip.eu.

The SEA-on-a-CHIP project has received funding from European Union's Seventh Framework Programme (FP7-OCEAN-2013) under grant agreement No.614168.

Notes

PP 45

Optimising the Removal of Steroid Hormones and Pharmaceutical and Personal Care Products (PPCPs) from Aqueous Media by using Low Cost Biosorbents

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With a growing global population, increased urbanization, and continually increasing use of pharmaceutical and personal care products (PPCPs), there is an increasing impact of Endocrine Disrupting Chemicals (EDCs) and PPCPs in wastewater effluents and receiving surface waters (1). Conventional treatment processes are not sufficient to remove such compounds from wastewaters (2), and as a result EDCs and PPCPs have been commonly detected in aquatic environments (3) at up to part per billion (ppb) concentrations in wastewaters and in receiving surface waters. Steroid hormones have been linked to reproductive disturbance and developmental problems in wildlife and humans at ultra-trace, part per trillion (ppt) levels, while the effects of exposure to PPCPs are less well characterized but may include environmentally acquired antibiotic resistance and other miscellaneous biological effects (4,5).

This project aims to evaluate the potential application of recycling industrial and agricultural by-products as low cost biosorbents for optimizing the removal of PPCPs and EDCs from aqueous media that have previously undergone secondary wastewater treatment. The absorbent is designed to be a final 'polishing' treatment to further effectively and efficiently remove any remaining compounds from a simplified matrix. Instrumental methods for the detection of 17 prioritised compounds by liquid chromatography tandem mass spectrometry (LC-MS/MS) have been developed. Eleven low-cost biosorbents derived from mainly Scottish industrial and agricultural wastes such as spent grains, crab shells, coffee wastes and algae, as well as a reference material activated carbon, have been evaluated for their ability to absorb the target analytes under laboratory conditions. The effectiveness of the biosorbents under natural environmental wastewater conditions (i.e. pH, ionic strength, temperature, existence of competing organic or inorganic, contact time and adsorbent concentration) were then studied. The economic feasibility of scaling up the most effective and efficient biosorbent systems to an industrial scale will be investigated with pilot studies at Scottish Water and the Chinese Academy of Sciences. It is anticipated that the dynamic treatment system will be applicable in real wastewater system in a fast, inexpensive, and sustainable treatment system.

This project is sponsored by the Scottish Government Hydro Nation Scholarship Scheme. Special thanks to Scottish Water, Scottish Environment Protection Agency and Centre of Expertise for Waters.

(1) Wang J, Wang S. Removal of pharmaceuticals and personal care products (PPCPs) from wastewater: A review. J Environ Manage 2016 11/1;182:620-640; (2) Rivera-Utrilla et al., Pharmaceuticals as emerging contaminants and their removal from water. A review. Chemosphere 2013;93(7):1268-1287; (3) Loos et al., EU-wide monitoring survey on emerging polar organic contaminants in wastewater treatment plant effluents. Water Res 2013 11/1;47(17):6475-6487; (4) Carlsson et al., Toxicity of 15 veterinary pharmaceuticals in zebrafish (Danio rerio) embryos. Aquatic Toxicology 2013 1/15;126:30-41; (5) Blanchfield et al., Recovery of a wild fish population from whole-lake additions of a synthetic estrogen. Environ Sci Technol 2015;49(5):3136-3144.

Notes

PP 46

Geochronological studies on sediment cores from Djerdap Lake - reconstruction of the pollution history

Gordana Gajica; Lukas Hagemann; Snežana Štrbac; Milica Kašanin-Grubin; Branimir Jovančićević; Nebojša Vasić; Jan Schwarzbauer

For geochronological studies in the Danube river system, the Djerdap Lake represents an important sediment archive. The largest single hydropower dam Djerdap 1 was constructed during 1972 on Danube at the Serbia-Romania border, at 943 km from the mouth. Building of the dam resulted in the formation of the Djerdap Lake, with a volume of about 3,500 million m3. Construction of the dam disturbed the natural equilibrium of Danube flow along that stretch, and induced impacts both in the backwater zone and downstream of the dam.

The objective of this investigation is a geochronological investigation of inorganic and organic anthropogenic pollutants in the Djerdap lake sediments (140 cm deep borehole, 11samples). Heavy metals, polychlorinated biphenyls, polycyclic aromatic hydrocarbons, pesticides, pharmaceuticals and personal care products were analyzed. Besides priority pollutants also source specific organic compounds (e.g. linear alkylbenzenes) were analysed as indicators for different emission sources. Based on the quantitative concentration profiles in the sediment archive a pollution history covering the beginning 1970'ies till today was reconstructed. Standard bulk properties, e.g. total organic carbon and grain size distribution was measured. The qualitative composition of the mineral part of the sediment was determined by X-ray diffractometer (XRD), and trace as well as rare earth elements were determined by atomic emission spectrometry with inductively coupled plasma (ICP-AES). Organic contaminants were analyzed by gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS) measurements after applying a standard extraction method (Accelerated solvent extraction-ASE) and subsequent fractionation by liquid chromatography on silica gel to appropriate sub samples.

Obtained results gave insight the pollution history of investigated lake sediments. They allowed not only to distinguish the impact from different emission sources (e.g. coal production, industrial emissions, sewage, agricultural run-off etc.) over time, but also to evaluate the long-term efficiency of past regulation measures or other influences on emission rates.

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