

January 2021 Environmental Chemistry Group

Bulletin



"Times of change: this edition has a special focus on online outreach and desktop events."

Desktop events. We report five desktop events. Jeremy Thomas extracts ideas from *ClairCity* Webinars; John Collins details the RSC *Environmental Science* journals desktop event; and Rowena Fletcher-Wood reports on one session from *Communicate 2020*, and the ECG's presence at *IF Oxford*, bringing outreach online. Laura Alcock summarizes #EnvChem2020, and #EnvChem2021 is announced.

Chair's Report. Tom Sizmur reflects on a challenging year, changes to the committee, and the success of our first online conference #Envchem2020.

Article. Karen Hudson-Edwards explores the resource potential of mine wastes.

Environmental Briefs. Symiah Barnett uses density analysis to distinguish microplastics. Jay Bullen shares surface complexation models to predict adsorption. Jamie Harrower delves into fugacity modelling. Daren Gooddy writes on phosphate oxygen isotopes for nutrient sources and cycling.

Also in this issue. Caroline Gauchotte - Lindsay tells us how she was sidetracked by analytical chemistry on her way to becoming a forensic scientist. Laura Newsome reviews *Soil Clays*. Rowena Fletcher-Wood reviews evaluation training by Jamie Gallagher. Our first Outreach Activity Sheet on filter funnel engineering is included.

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Report **Chair's report for 2020** Tom Sizmur (University of Reading, t.sizmur@reading.ac.uk)

As many of our members will appreciate, 2020 has been a challenging year – and these challenges have not escaped the Environmental Chemistry Group.

Our first event of the year, the **Early career researchers' meeting** on March 11th, was also our last to be held 'in person'. The meeting, which included presentations from outstanding early career environmental chemistry on subjects spanning the environmental chemistry of water, sediment, soil, and air, provided an opportunity for us to practise the valuable skill of greeting one another using elbow bumps. We are especially grateful to **Dr Laura Carter** (University of Leeds) and to **Antony Poveda** (Mangorolla CIC) for presenting keynote addresses, and congratulate **Chinonso Ogbaugu** (University of Reading) and **Fereshteh Hojatisaeidi** (London South Bank University) for winning the prizes for the best oral and poster presentations, respectively.

Many of our plans for events in 2020 have been postponed, including our **Distinguished Guest Lecture and Symposium** on **Electronics in the Environment** and collaborative events on **Plastics, From Cradle to Grave**

and Resurrection and Sensors and Networks for Environmental Monitoring. We have tentative plans to reorganise these events either online or in person.

In July, we planned to hold a twoday **#EnvChem2020** (see **page 9**) conference hosted at the University of York as part of our **#EnvChem**

series: this annual event is planned as mobile, visiting different venues every year. After much debate, we hosted an online meeting using Zoom in partnership with the Society for Environmental Toxicology and Chemistry (SETAC), and made this event free of charge to both members and non-members. The response from our community was immense, with 48 abstracts received and more than 350 delegate registrations. We are particularly grateful to **Professor Iseult Lynch** (University of Birmingham) for providing an excellent keynote presentation on the ecotoxicology of nanoparticles in the environment. In an attempt to encourage online interactivity and replicate some of the networking made possible at an in person conference, alongside presentations made in the 'main room', we ran 13 parallel breakout rooms, where delegates viewed and discussed shorter presentations, similar to a poster session. While I would be lying if I claimed the event went without a hitch, with extraordinary effort we were able to overcome many of the challenges, and the feedback from delegates was overwhelmingly positive. We were particularly pleased that the event had a more international reach than originally expected. A special issue of the science presented at the meeting is being prepared for publication in **Environmental Toxicology and Chemistry**. Plans are also underway to enhance and host **#EnvChem2021** online again in July.

For the last few years, the Environmental Chemistry Group has provided a stand at the **IF Festival of Ideas**, in Oxford, as part of a programme of activities we undertake to support science engagement and outreach. This year, the festival went online, and we provided video and written materials demonstrating chemistry experiments that children of all ages can undertake at home during lockdown (see **page 21**), now a rich legacy resource of material that can be used by families and teachers.

I also report a few recent changes to the committee. At the start of the year, we welcomed **Dr John Collins** (Environment Agency) and **Dr Tomás Sherwen** (University of York) onto the committee. At the end of the year, we said goodbye to our **Secretary Dr Glynn**

"2020 has been a challenging year – and these challenges have not escaped the Environmental Chemistry Group." **Skerratt** and our Bulletin production editor, **Dr Clare Topping.** Glynn has provided invaluable support to the committee and me in particular over the past 2.5 years, ran the hugely successful meeting on **Sustainable water in the 21st century** in 2019, and has authored multiple Bulletin articles. Clare coorganised the inaugural **Plas-**

tics: From cradle to grave, and resurrection meeting in 2019 along with the RSC's Toxicology and Food Groups, and the Society of Chemical Industry (SCI). A follow-up event is planned for 2021. Clare also took on the monumental task of copy-editing and formatting the Bulletin as its Production Editor. I wish both Glynn and Clare all the best in their future endeavours. We are enormously grateful for their contribution to the committee.

We have rotated other roles on our committee: **Professor Steve Leharne** has taken over the position of **Secretary**, and **Dr Rowena Fletcher-Wood** succeeds me as the **Chair** (while I move to the position of **Vice Chair**). **Dr David Owen** has taken on the role of representing the ECG on the RSC's committee of the Environment, Sustainability and Energy Division.

I would like to take this opportunity to wish you a safe and prosperous 2021.

The ECG Interview: Caroline Gachotte-Lindsay

Dr Caroline Gauchotte-Lindsay is a Senior Lecturer in Water and Environmental Engineering at the University of Glasgow. She specialises in developing novel analytical solutions to monitor and remediate pollutants.

What inspired you to become a scientist? When I was

12, I took a keen interest in genetics;

one day, I read about its use in forensic science in the kids' science magazine my granddad had bought me a subscription for. It was the very beginning of the use of DNA in police investigations in France. From then, I decided I wanted to be a forensic scientist (this was before CSI!) and it guided my choices in the subjects I studied.

How did you come to specialise in environmental analytical chemistry? On my way to becoming a forensic scientist, I discovered analytical chemistry. I realised that chemistry was even more exciting to me than biology (my Cartesian side, I suppose), and so pursued my postgrad education in analytical chemistry. During my PhD, I joined a civil engineering department where I got hooked on environmental forensics (attributing contamination events to their polluters). The environmental dimension involved much more complex matrices, and to me that brought exciting challenges.

Could you describe your current job? I am a lecturer and a researcher in the James Watt School of Engineering at the University of Glasgow. I teach chemistry and environmental engineering to civil engineering students, which is a great challenge! I also have a diverse and talented research group. We investigate new ways of measuring organic compounds in many environmental matrices by combining advanced analytical methods with machine learning. Finally, I also do citizenship work for the University and the wider community, mostly around gender equality in STEM subjects.



What advice would you give to anyone considering a career in environmental chemis-

try? Do it: we need you! I would also advise you to cultivate a taste for interdisciplinarity. The environment is complex, and chemistry must team up with numerous other fields to tackle it.

What are some of the challenges facing the environmental chemis-

try community? The main challenge for me is that some of the issues we tackle as environmental scientists have become urgent: climate, water scarcity, atmospheric pollution. We need to act fast but also smart, and sometimes the two don't go together well. We also must keep advocating for all issues, even when the general public focus is on "pet" issues such as plastic pollution.

What is the most rewarding aspect of your career so far? I wouldn't work in academia anymore if it wasn't for the most rewarding part of my job: enabling others in their careers. Undergraduates graduating, PhD students defending their hard work, postdoctoral researchers moving on to permanent jobs – this is what keeps me going.

If you weren't a scientist what would you do? Good question! I have multiple interests; science was never the only option. Back when I was a teenager, plan B was to be a high fashion stylist. Now I think I would want a job where I can directly impact people's quality of life, maybe a politician or a midwife!

And what do you do when you are not working? Nowadays, mostly being a *maman* to my little girl, although now that she is a little bit older, I am also back to hiking in the Scottish hills – now with her. I also do crochet and cross-stitching, and I am currently learning Italian.

Review

Evaluation training – Dr Jamie Gallagher

Rowena Fletcher-Wood (Freelance science communicator, rowena.fletcherwood@gmail.com)

and in person.

Dr Jamie Gallagher is an award-winning the truth could not be more different: if they are left to engagement professional specialising in read or think later, few participants will; meanwhile, impact narratives and evaluation. Along-or corrected by the training provider, are more readily side his successful Periodic Table Show, encoded into our memories. Moreover, by encouraging he partners with other institutions to train critical thinking he established an understanding of practitioners in public engagement with content that is rarely accessed in lecture format. Howevresearch skills. This review focusses on the function for multiple or multin or multiple o his Evaluation training for public engage-audience and immerse them in the material - and lecture, ment activities, which is delivered online which is substantially less effective. As such, his Lord of the Rings analogy for choosing the right "ring carrier" remains most fresh in my mind - but I may be a biased

Dr Gallagher began the workshop with a clear outline of audience, as I had heard it before. His training made some key terms and concepts within which he was effective use of case studies and group work, supported operating, so as to best identify the aims and metrics for by platforms such as his own website and Google Sheets success for the workshop - or, in other words, teaching (the latter trialled for the first time during this session),

by example.

Through mastery of technology (including "hold music" and "holding slide") and opening the online space early, Dr Gallagher created a professional feel for the training. In addition, two inbuilt tea and coffee breaks kept participants refreshed and active, and overall contributed to a positive training experi-



Figure 1. Define your initial terms to ensure evaluation data is meaningful.

which were seamless in application.

Evaluation tools approached were with a critical eve, and the training not only identified methods for gathering evaluative data (albeit a limited subset of the wide range of available tools), but also invited us to analyse choices

ence across his three hour workshop.

including breakout rooms, messages, and question- solutions to problems such as flatlining (where formtaking. Alas, he found reading and speaking simultane- fillers tick down a vertical line without reading the ously somewhat challenging, leading to lengthy silences questions alongside). As anyone who has worked with during which the presenter's eyes scanned from left to teenagers will be aware, use of technology to identify right as he rapidly assimilated the chat content and smiling and frowning faces is a poor measure of impact: sporadically brought up relevant points or queries. The Dr Gallagher pointed out that happy people can frown training involved plenty of interactivity. Academics often and unhappy people can smile, and so this constitutes

and identify potential bias, such as voting stations that use plastic counters and are subject to bandwagonning Throughout, he continued to use a range of online tools, (swaying voters towards the trend), or offering practical feel that this is a less efficient use of workshop time, but poor evidence for enjoyment. In fact, as he might have

"Most evaluation is

totally awful and

completely pointless."

added, when concentrating and taking in information, most people wear a blank expression. Dr Gallagher showcased both qualitative and quantitative tools, and did not confine his recommendations to 'hard science' metrics, including methods such as thematic analyses which are traditionally employed by the social sciences and executed upon social media or other unregulated

sources. Where testimony is concerned, expert testimony may be more meaningful than individual testimony, but individual testimony can provide colour to evaluation when supplied alongside quantitative analyses.

Dr Gallagher drew extensively on the RSC's Public attitudes to chemistry research report, and reported on its finding as they pertained to evaluation. This research, carried out in 2015, constitutes a comprehensive examination of what the public understand by the term "chemist" and the role of chemists in society. Notably amongst their findings was the ingrained identification of a *chemist* as a *pharmacist* - suggesting that past evaluation data that assumed understanding of this difference may be invalid. Findings concluded that avoiding the term chemist and instead discussing scientists who worked on chemistry was far more effective for eliciting helpful responses than attempting to change public perceptions. Also pivotal in the report's findings was that whilst chemists expected public perceptions of them to be negative, they were actually neutral. These unexpected outcomes have since formed core learning material in the field of evaluation, especially chemistry.

"Most evaluation is totally awful and completely pointless", Dr Gallagher declared. Many evaluators begin without clarity of purpose, their evaluation may not be proportionate to their engagement, and they may not consider how questions may be misinterpreted or what they, the evaluators, will do with answers. Every question should serve a purpose. Indeed, in the charity sector, the term "theory of change" is used to describe the backward logic model by which you begin with your final outcomes and work backwards to identify the steps needed to achieve those; evaluation should be no different. That is, questions should be asked to obtain the information needed, rather than chosen randomly and their insights later extracted. If your purpose is to improve your work or your outreach, sidestepping evaluation practices and simply asking your audience may be a better solution. If you are running a one-off project, the number of respondents and integrity of data may not be sufficient to be worth your time - and reflection after the event is one potential alternative.

Demographics and diversity were discussed, from the prevalence of old white men in science to gathering demographic information on children: the demographics of your chosen speakers, organisers and event managers could inform the visibility of diversity in science, whilst the gender of children attending can be difficult to capture and may not be essential infor-

mation.

Towards the end of the training, timing must have gone awry; slides were rushed, so we only briefly discussed critiquing evaluation form questions and

avoiding fundamental errors such as the use of "and" – which can transform a simple yes/no question into a complex one, where the respondent partially agrees and partially disagrees, especially in the absence of the "don't know" option.



Figure 2. Misuse of "and" can transform a simple yes/no question into a complex one, especially in the absence of the "don't know" option.

Overall, Dr Gallagher's training provided valuable tools for in depth evaluation analysis and critique, prioritising thinking skills that allow the individual to consider their choices over breadth in the field and core information that constitutes the bread and butter of evaluative best practice. His workshops might make a poor introduction to the field, but excellently upskills practitioners who wish to take ownership of best practice science communication.

Resources

You can find out more about Dr Gallagher and the training he offers at www.jamiebgall.co.u, and read the *Public attitudes to chemistry research report* at https://www.rsc.org/globalassets/04-campaigning-outreach/campaigning/public-attitudes-to-chemistry/public-attitudes-to-chemistry-research-report.pdf

Book Review Soil Clays

Laura Newsome (University of Exeter, I.newsome@exeter.ac.uk)

What can we gain from knowledge of soil clays? This book seeks to answer the question and to impart that knowledge. Targeted towards soil or environmental scientists, agronomists and/or land planners, *Soil Clays: Linking Geology, Biology, Agriculture and the Environment* is a useful reference book for understanding more about the critical zone that sustains terrestrial life on Earth.

The number of humans on Earth has increased immensely during the last century and will continue growing for the foreseeable future. To feed the world's population, it has been estimated that soils need to provide 50% more food. Not only this, soils provide physical support and nutrients for plants, mitigate flood waters, stimulate the breakdown of organic matter and wastes, store carbon dioxide, and are a habitat for micro- and macrofauna and the microorganisms that provide element

biogeochemical cycling. But, why clays? The central proposition of this book is that "major properties of soils can be reduced in a large part to those of their clay minerals". To understand soils, we need to understand soil clays.

years ago when vascular land plants with deep roots evolved, contributing to physical, chemical, and biological weathering.

Chapter 2 introduces the mineralogy of sheet silicate minerals, assuming some prior knowledge, and describes how cation substitution, interlayer anions and vacancies arise and lead to charge deficiencies, influencing chemical behaviour and thus the availability of nutrients. The chapter would benefit from a list of general chemical formulae for the different mineral groups, and a glossary.

Of most interest to environmental chemists, is Chapter



6 – chemistry of alteration by weathering. Here, interactions are described between primary minerals and protons derived from rainwater and/or electrons derived from dissolved oxygen. These cause weathering by mineral change, dissolution, diffusion, ion exchange, and oxidation. Chemically stable aluminosilicate minerals rapidly precipitate from solution, and are therefore common solid-phase products. In contrast, ionic alkali metals and alkaline earth metals are more soluble. Chapter 7 describes the mechanisms

of clay formation (*e.g.* crystal growth and thermodynamic considerations). Chapter 8 is an excellent reference source for the nature and origin of secondary clay minerals, while Chapter 9 covers the effect of different climates on soil clay formation.

The book describes soils as weathered from rock, Chapter 10 reviews the literature on the interactions between soil clay minerals and organic matter, which

supporting (or capable of supporting) life, 🖌 porous, and forming horizons; clays as secondary inorganic materials less than 2 µm in size. Although rocks have been weathering since the atmosphere became oxygenated 2.4 billion years ago, soils only formed 440 million



bv selective react adsorption and surface polymerisation. Importantly for carbon turnover dynamics, clays can sequester organic matter away from soil organisms that would otherwise consume it and release it back to the atmosphere as carbon dioxide. Chapter 10 also

covers the concepts of soil micro- and macroaggregates tion by clays and medicinal clays is included. Given their (Figure 1). Microaggregates are poorly described as importance, more details would have been useful. The

"the fundamental units of soils". They are associations of organic matter with phyllosilicate and oxide minerals, which are a few μm in size, and with varying compositions and shapes. Given their importance, it was disappointing the book did not contain a good diagram, such as Figure 1.

Chapter 11 and 12 review how soil clays can be extracted and identified, and are better suited to

vantages and disadvantages of techniques.

The effects of surface charge, surface area and particle **References** size are covered in Chapter 13. My understanding is that the large surface area and strongly charged surfaces of clays explain why they are so reactive. Placing this chapter towards the end of the book is therefore out of place.

If you were still wondering, why clays matter, then Chapter 14 outlines their role in agriculture, environment, and society. This includes how soil clays support plant nutrition, hold water, impact buildings by shrinking or swelling, and sequester carbon. Pollutant mitiga-

"Clays can sequester organic matter away from soil organisms that would otherwise consume it and release it back to the atmosphere as carbon dioxide."

final chapter summarises the

entire book in just 12 pages. If you have limited time, this is a great place to start.

In summary, clays are sometimes forgotten or not considered because they are too small, thought to be insignificant, or too difficult to understand. This book argues the case for clays, explaining what they are and the mechanisms for their chemical reactivi-

specialists. They could be improved by outlining ad- ty. It is a useful reference material that unifies all aspects of soil clays.

- 1. Churchman, G. J. and Velde, B., 2019. Soil Clays: Linking Geology, Biology, Agriculture and the Environment. 1st Edition. CRC Press, Boca Raton, FL. ISBN: 9781498770057.
- 2. Additional reading: Jastrow, J. D. and Miller, R. M., 1998. Soil Aggregate Stabilization and Carbon Sequestration: Feedbacks through Organomineral Associations. In Stewart, B., Lal, R., Kimble, J., Follett, R., Stewart, B. (Eds.). Soil Processes and the Carbon Cycle. CRC Press, Boca Raton, FL. ISBN: 9780203739273.

Upcoming meeting #EnvChem2021: Chemistry of the whole environment (online)

Following the successful #EnvChem2020 event held last July at the height of the Covid-19 pandemic, we announce our research conference #EnvChem2021, which will also be held online on Friday 25th June.

#EnvChem2021 provides a forum for early career and established researchers working in environmental chemistry and ecotoxicology to share their latest research. This meeting, organised by RSC Environmental Chemistry Group will comprise a programme of presentations from delegates who submit abstracts in the following themes:

- Environmental processes in soil, water and air
- Emerging contaminants
- Novel techniques
- Atmospheric chemistry
- Ecotoxicology

Registration

Registration is free of charge. You can register online by 3rd May 2021.

Call for abstracts

We request abstracts in the themes listed above. A template and contact details will be provided on our website: https://www.envchemgroup.com/upcoming -meetings.html

Abstract deadline: 3rd May 2021.

Meeting Report #EnvChem2020: Chemistry of the Whole Environment Research

Laura Alcock (Edwards Ltd, laura.alcock@edwardsvacuum.com)

"The proceeding discus-

sion highlighted the im-

portance of singlet oxygen

in the atmosphere, which

is produced in high

concentrations. compared

to other ROS. and shows

higher quantum yields."

This one-day conference was jointly organised by the ECG, and UK Branch of the Society for Environmental Toxicology and Chemistry (SETAC).

Intended to take place in York, #EnvChem2020 was our first online event. Despite technical challenges such as the reorganisation of face-to-face posters, this successful event allowed participation from far-spread delegates. The format involved nine speakers delivering 15 minute presentations, and a key-note. Posters were delivered as flash (three minute) presentations in "breakout" rooms.

Main presentations

Michelle Bloor chaired the first session, introducing **Dr Nadine Borduas-Dedekind** (ETH Zurich). Dr Borduas-Dedekind's presentation *Reactive oxygen species (ROS), including singlet oxygen, production within irradiated aqueous organic aerosols* began with a Zurich sunset, which represented a variety of atmospheric chemistries including photochemistry, cloud types, and

industrial emissions. Dr Borduas-Dedekind covered the formation of singlet oxygen, exploring its inlaboratory generation using organic aerosols. Analysis was achieved by filtration and dissolution. Probe decay was used to measure singlet oxygen over time and liquid chromatography for total organic carbon. Quantum yields were calculated to normalise steady state concentrations using liquid chromatography-UV/visual light spectroscopy, which compared well to aquatic environments. The proceeding discussion highlighted the importance

of singlet oxygen in the atmosphere, which is produced in high concentrations, compared to other ROS, and shows higher quantum yields.

Ayushi Priyam (Deakin University) next presented *Investigation for ecosafety and transformation of phosphorus based nanofertilisers by using* Caenorhabditis elegans *as a terrestrial model.* The presentation focused on the effects of nano-fertilisers on *C. elegans.* Uptake of nano-hydroxyapatite was monitored by fluorescent isothermal titration calorimetry (ITC) tagging. Different methods of producing the nano-fertiliser resulted in different shapes and sizes of the products and, whilst all formulations had a minimal effect on the survival of organisms, rock phosphate showed the greatest impact. The study determined that nanofertiliser formulations had a greater biocompatibility than bulk rock phosphate; thus, provided the correct compound is selected for the application, they cause less detriment to the environment than bulk fertilisers.

Jamie Harrower (Glasgow Caledonian University) closed the first session with a presentation on *Monitor-ing antibiotics in urban river environments using in-situ calibrated Polar Organic Chemical Integrative Samplers (POCIS), grab sampling and analysis by SPE-LC-MS/MS.* POCIS samples were collected at accessible points upstream and downstream of a wastewater treatment plant (WWTP) in Scotland and were calibrated over a 12 day period. Factors affecting function were identified and, where possible, mitigating actions taken. Monitoring demonstrated that the WWTP effluent contained high concentrations of pharmaceutical compounds, especially penicillin, and highlighted potential contamination by landfill sites. Proposed further

work includes comparison to river sediments, using fugacity modelling (see **page 29**).

Dr Rowena Fletcher-Wood chaired the second session and introduced the keynote speaker **Professor Iseult Lynch** (University of Birmingham) who spoke on *Multi-generational assessment of nanomaterials (NMs) toxicity: particle ageing reduces toxicity and ageing effect of the NMs on*

D. magna. Water fleas (*D. magna*) rely on an ecocorona, composed of a wide range of biomolecules, that affect what can bind or be combined within it. A selection of nanomaterials were introduced to the environment. Agglomeration of the particles increased uptake by *D. magna*, as no significant uptake of particles < 50 nm in diameter was observed. The impact of nanomaterial exposure on the brood, generational timelines and brood survival rates were explored. Initial exposure to uncoated TiO₂ prevented reproduction entirely. The exposure concentration was reduced,

"Fertiliser usage

accounts for over 85% of

all atmospheric release of

ammonia in western

countries."

resulting in successful reproduction, but significantly lower brood survival rate. Dissolution and accumulation of the nanomaterials, and the growth and reproduction of *D. magna*, including changes in morphology, were also discussed. Accelerated ageing was observed. Gene expression changes resulted from nanomaterial exposure, and protein corona differences were examined. Professor Lynch concluded that the effects of aged nanomaterials on the *D. magna* were significantly less severe than that of new materials. Natural organic matter reduced the surface energy of the nanomaterials. The presence of nanomaterials did not simply result in oxidative stress in the *D. magna*, but also in accelerated ageing.

John Collins chaired the first afternoon session and introduced **Oluseun Sunday Olubode** (University of Ibadan), who presented on *Allelopathic effects of* Celosia trigyna L. *on germination and growth of three widely cultivated African indigenous vegetables in Ibadan, southwest Nigeria.* Dr Olubode outlined how solutions extracted from the shoots and roots of the weed (C. *trigyna*) were prepared across a range of concentrations (0, 12.5, 25, 37.5, 50 gL⁻¹) and applied to 30 seeds per plant. Germination rate was then assessed 2, 4 and 6 days after sowing. Germination was found to be inhibited by treatment, whilst the shoot extract stimulated germination. Plumule and radicle growth were also assessed, with the shoot extract promoting plumule growth and inhibiting that of radicles.

Alexandra Richardson (King's College London) then

presented Using LC-MS, passive sampling and predictive modelling to understand the occurrence and environmental impact of contaminants in a London urban river system. There was a particular focus on contaminants of emerging concern (CECs; pharmaceuticals, pesticides and personal care products), the seasonal changes in these contaminants, and predicting

the bioconcentration factor in invertebrates by machine learning. Ms Richardson outlined the methods of sample collection during summer and winter sampling campaigns. Sample extracts were prepared and analysed by reverse-phase liquid chromatography coupled to a quadrupole-time of flight (Q-TOF) method and a reversed-phase biphenyl coupled with a rapid quadrupole (MS/MS) method – particularly for water samples. All samples were compared to a set of 164 standards and 34 CECS were found in the winter water samples, compared to 53 in the summer water samples. 58 CECs were found in the winter passive sampler extracts, compared to 67 in the summer. A four-layer perceptron-based machine learning model for predicting the bioconcentration factor in Gammarus pulex was applied. Following training, optimisation and testing, the model achieved an R² performance of 0.98 and 0.91 for verification and blind tests, respectively and externally

validated using experimental data from animals. The different numbers of CECs found in Thames river water between winter and summer were attributed to differences in the resident population of London during the two periods. The most prevalent compounds were selected for bioaccumulation testing.

Aoife Quinlivan (University of Nottingham) finished the session by presenting Preventing the rising tide of AMR: Utilising stable water MOFs to remove antibiotics from wastewater. She identified anthropogenic water pollution as a primary contributor to antimicrobial resistance (AMR) within the environment and explored the stability and effectiveness of metal-organic frameworks (MOFs) for removing CECs from water. Current WWTPs are not equipped to deal with antimicrobial compounds. MOFs consist of metal anodes connected by organic linkers, giving them high structural porosity. They have a large surface area, resulting in a high capacity for adsorption; their linkers can also be functionalised, allowing for specification and selectivity to prevent removal of desirable compounds from the water, whilst maximising removal of the target compounds. Ms Quinlivan presented criteria for industrial viability and functionality, with an overview of the specific MOF - MIL-100 (Fe), synthesised by microwave irradiation and then characterised. She outlined MIL-100 (Fe) stability as a function of time, temperature and quantity of adsorbent used to remove ciprofloxacin from water. Following each test, the MOF was centrifuged and dried. Functional groups were identified and pH monitored over time, giving a rapid initial

drop. Stability was affected by seasonal temperature, which may affect industrial applications. There was a logarithmic relationship between the relative masses of the MOFs and the pH of the water matrix. Water containing ciprofloxacin was dosed with MIL-100 and analysed, at incremental time periods, by liquid chromatog-

raphy-mass spectroscopy (LC-MS). Over time, the concentration of the antibiotic compounds within the water samples decreased.

Dr Tom Sizmur chaired the final session of the day and introduced **Jize Jiang** (University of Edinburgh), who presented on *Developing a climate-dependent model of ammonia emissions from agriculture discussing human impact on the nitrogen cycle, through agricultural emissions of ammonia*. Fertiliser usage accounts for over 85% of all atmospheric release of ammonia in western countries. Temperature and water interactions significantly impact ammonia volatilisation, calling into question official ammonia emissions values, based on the calculation of these figures from statistical data with limited analysis of meteorological data. Mr Jiang's model aimed at providing more reliable estimates of ammonia emissions, considering meteorologi

cal effects like temperature, relative humidity and pH, and temporal variations. Chicken farming was used as a model, requiring the collection of detailed ammonia emissions data. The model considered global emissions of ammonia from chicken farms and calculated that the highest emissions would occur in tropical areas of high temperature and humidity. Conversely, hot, dry areas were predicted to produce much lower emissions. Mr Jiang and his colleagues next plan to quantify emissions from other livestock sources and develop a bidirectional exchange model. His answers to questions highlighted the fact that the most significant factor in agricultural ammonia emissions is human management.

Alberto Celma (University Jaume I of Castelló) then delivered a presentation on The combination of bioanalyses with ion mobility high-resolution mass spectrometry for an enhanced environmental screening. His project combined in vitro bioassays with chemical analyses to identify the presence of organic contaminants within coastal lagoons across Spain's Mediterranean coast. High resolution mass spectrometry (HRMS) and ion mobility separation (IMS) were employed for widescope analysis, and prior separation of the analyte. Coupling these techniques provides huge scope and resolution, but unwieldy datasets. The team also carried out a series of eight bioassays. Results were combined with target and non-target analysis by IMS-HRMS. The different toxicity profiles of the samples allowed identification of a range of organic contaminants present in the lagoons' surface waters, as well as identifying an influence on anomalous data, in the form of WWTP effluent.

Qingzhe Zhang (Institut National de la Recherche Scientifique; INRS) provided the final presentation of the day in which he identified environmental pollution and energy demand as two primary threats to human life and proposed the use of photocatalysts to address both in his presentation Broadband solar harvesting via plasmonic and heterojunction nanostructures for environmental and energy applications. Mr Zhang explained that photocatalysis could directly harvest and utilise solar energy and addressed the challenges of this application: many photocatalysts only interact with ultraviolet (UV) and blue light, leaving much of the incident solar energy unused. The focus of the study was increasing solar energy usage for remediation of environmental samples. Plasmonic gold (Au) particles were incorporated into a semiconductor to improve photocatalytic efficiency using the "size-tuneable" localised surface plasmon resonance effect of the gold nanoparticles (AuNPs). These were then tested in the remediation of organic contaminants in wastewater samples. Lanthanide-doped NaYF₄ (NYF) coupled with graphitic carbon nitride $(g-C_3N_4)$ AuNPs were stable and demonstrated improved photocatalytic activity, using UV, visible, and near infrared (NIR) light to degrade organic pollutants. AuNP-loaded hierarchical TiO₂ spheres also showed "strikingly high activity and selectivity" for the reduction of 4-nitrophenol to 4aminophenol with visible light radiation. However, as Mr Zhang highlighted, gold and rare-earth metals are expensive. To improve efficiency and cost-effectiveness, and

reduce environmental toxicity, a 0D/2D heterojunction was constructed, based on NIR-responsive quantum dot (QD) loaded g- C_3N_4 nanosheets. These exhibited the highest recorded photocatalytic activity in wastewater treatment.

Breakout room presentations

Dr Aaron Schultz (University of Alberta) presented *Trouble Relaxing: polyacrylic acid coated nanoparticles impair blood vessel physiology.* This was the first study to use an *ex vivo* perfusion method, mimicking circulation, coupled with dual-wire myography to study the effects of nanoparticles on the circulatory system. Iliac arteries from cane toads were perfused with polyacrylic acid-coated TiO₂ nanoparticles, which inhibited Ach-mediated vasodilation by approximately half, attributable to damage to the epithelial layer of the lumen in the vessels.

Dr Adam Peters (WCA Environment) presented two talks. The first; Implementation of environmental quality standards for bioavailable metals: Compliance assessment, discussed the challenges faced by regulators, including numerous locations, additional resources and expertise, and the measurement of parameters other than bioavailability of metals. The second, Demonstrating the reliability of bio-met: A simple bioavailability tool for determining compliance with Environmental *Quality Standards (EOS) for metals*, introduced a simplified model, based on a Biotic Ligand Model for implementation of bioavailability-based EQS in European freshwaters. In a suitability study, over 80% of the predictions fell within a factor of three of the experimental findings and 99% of predictions were within a factor of two. Further validation using a larger set of European natural water samples, demonstrated reliability "over a broad range of water chemistry conditions".

Dr Balal Yousaf (University of Science and Technology of China) presented *Role of biochar application on environmental transformation and fate of engineered nanoparticles (ENPs) in soil-plant system.* Biochar material was produced and added to soils to immobilise TiO₂ ENPs and reduce bioaccumulation of Ti in wheat plants. Testing showed that biochar cut the Ti concentration in wheat tissues by two thirds and the transfer rate reduced by 50% when plants were exposed to the highest concentration of Ti ENPs (1000 mg L⁻¹).

Dr Ben Maskrey (Cefas) presented *Seasonal occurrence of pharmaceuticals and related compounds in bivalve molluscs from England and Wales*, reporting the bioaccumulation of active pharmaceutical compounds in oysters and molluscs collected from six sites across at four points throughout the year. Antidepressants, particularly sertraline, were identified. Seasonal and site-specific fluctuations were observed.

Bilikis Folarin (University of Lagos) delivered *Antibiotic residues in chicken muscles and eggs purchased from poultry farm and local market in Lagos, Nigeria.* This study investigated the presence of ciprofloxacin, oxytet-

racycline and tetracycline, used for food hygiene purposes in poultry farms. All three compounds were present at concentrations above the maximum residue limit (MRL) set by the Food and Agriculture Organisation of the United Nations. Ciprofloxacin was highest in thigh meat, oxytetracycline and tetracycline in eggs.

Brian Durham (University of Birmingham) presented *Carbon dioxide/water/ice equilibria at atmospheric partial pressures.* Following a conceptual model of crystal growth, modified to account for gas hydrate for-

mation, the project team intend to continue to grow " CO_2 frost" in vitro, utilising pure reagents to obtain empirical data on CO_2 molecule behaviour at the ice phase boundary.

Celine Moreira (Polymateria Limited) delivered *Biodegradable plastics: a compatible approach to solving short- and long-term associated risk of*

plastic contamination in countries of the Global South. In this talk, the scale, challenges and hazards associated with plastic waste, including types and overall availability of biodegradable plastics were presented.

Christopher Howick (INOVYN Chlorovinyls Limited) discussed *The importance of nomenclature in the under-standing of chloroalkanes* linking measured chlorination level and chain length found in matrices and articles to primary raw materials, His presentation linked the difficulty of manufacturing chloroalkanes to appropriate standards, due to their high isomeric content. Developments in the analysis of these compounds has led to updated standards and regulations.

Chris Hughes (Ricardo Energy & Environment), spoke on *Advances in bioavailability science and application to chemical regulation*, and discussed the role of bioavailability in determining the risks presented by chemicals within the environment. He also discussed the risks associated with failing to consider the fate of chemicals or the concentrations that they can reach in the environment. This can cause under- or over-estimation of the potential risks, hazards and exposure.

David Brown (Ricardo Energy & Environment) discussed *Challenges and learnings from biodegradation testing of complex and difficult test substances.* Challenges include unknown or variable composition, complexity of reaction products, biological materials, and testing limitations. Hydrocarbons, for example, are unsuitable. Development and validation are needed, especially since false negatives could have significant regulatory, classification and, as a result, environmental consequences.

Godswill Tesi (Federal University of Petroleum Resources) spoke on *Organochlorine pesticides (OCPs) in agricultural soils of Southern Nigeria: Spatial distribu-*

Christopher Howick's presentation linked the difficulty of manufacturing chloroalkanes to appropriate standards, due to

their high isomeric content.

drin.

Harrison Frost (University of Surrey) discussed *The Ad*sorption of aqueous metal(loid)s by microplastic fibres: Preliminary findings. Adsorption of 12 metals and metalloids onto polyester fibres were initially investigated, with 90% removal of Cd. Adsorption rates showed poor repeatability. Antimony

repeatability. Antimony leaching from the fibres was observed and attributed to the use of SbO_3 as a catalyst during polyester production.

Iain Wilson (WCA Environment) discussed Addressing the challenges associated with applying bioavailability-

based standards for metals in freshwaters. He highlighted the complexity of bioavailability models and the low availability of the required parameters as the primary difficulties. When combined with bio-met (https://biomet.net, a European industry-funded database initiative, he delivered new regional and ecologically relevant standards for Zn in French surface waters.

tion, source identification, ecotoxicological and human

health risks assessment. His study investigated 20 OCPs

in 18 soil samples from six locations. Total concentra-

tions ranged from 5.8 to 395 ng g-1, typically Chlordane

> HCHs > DDTs > Endosulfan > Endrin > Aldrin > Diel-

James Dinsley (University of Manchester) discussed *Uranium and lead uptake and transfer within plant-fungal symbioses.* This study investigated the use of plants and fungi for bioremediation of abandoned mining sites contaminated by heavy metals and naturally occurring radioactive materials (NORMs), with a focus on plantmicrobe interactions. The primary concern is the risk of transfer and bioaccumulation.

Janine Elliott (Scottish Environmental Protection Agency) presented *Chemical screening of surface waters – A proof of concept study.* She selected 13 locations, including agricultural, urban, forestry and semi-natural typologies, whereupon 135 non-target compounds were identified and 99 quantified, including some previously unobserved. Most were pharmaceuticals and their metabolites. Patterning was attributed to chemical usage. The tool shows potential for use in incidents where the source of pollution is unknown.

Dr Kirit Wadhia (National Oilwell Varco) delivered *Risk based assessment and regulatory drivers*, where he discussed the variation in risk endpoints by different oil and gas producers, based on the assumptions and input parameters used (only aligned in their use of chemical guidance values). He proposed a global regulatory framework to enable uniform risk assessment and comparable outcomes between companies.

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Lorraine Hutt (Environment Agency) spoke on *Identifying emerging contaminants in the environment: Development of the Environment Agency's PEWS scheme,* proposing a system to allow prioritisation of emerging contaminants for regulatory management based on potential risks to wildlife and the environment (the new Prioritisation and Early Warning System (PEWS)). The system considers the levels and patterns of chemical use, occurrence in the environment, potential hazards, evidence of impact, and the level of confidence in data. An appeal was made for people willing and able to provide additional data.

Megan Griffiths (Ricardo Energy and Environment) presented *Bioavailability, complex substances and overall persistence (BCOP): three themes to deliver a step-change in persistence assessments – Overview of a CEFIC-LRI project (ECO52).* She proposed significant improvements to guidance, especially for difficult-to-assess substances by considering bioavailability, providing guidance for complex substances, and incorporating overall persistence using multimedia fate models.

Michael Eze (University of Göttingen), discussed *Metagenomic insight into a diesel-degrading consortium for the bioremediation of diesel fuel contaminated sites.* His potential solution to expensive and "environmentally unfriendly" traditional methods for remediation of fuel contaminated land and soils was plant-microbe symbiosis, which proved a cost-

effective, eco-friendly bioremediation method. The study has also provided insight into the genes involved in diesel fuel degradation by plants and microbes.

Shivender Singh Saini (Central University of Himachal Pradesh) presented *A simple, self ensembled, chitin based sam*-

ple preparation approach for trace analysis of 17β estradiol in water. The method presented is simple, cost-effective and eco-friendly. Testing indicated good linearity in the 0.05 – 20 ng mL⁻¹ range and a lower detection limit of 0.02 ng mL⁻¹. It is hoped the method can be applied to other emerging contaminants in future.

Shweta Gelhout (The Energy and Resources Institute) delivered *Phytotoxicity assessment of mycosynthesized iron oxide nanoparticles on* Oryza sativa (*Asian Rice*) *in different soil types.* Iron oxide nanoparticles (n -Fe₃O₄) were synthesised with a verified biogenic approach. The role of the nitrate reductase enzyme during synthesis was investigated and the effect of biogenic n-Fe₃O₄ on *O. sativa* and plant-growth-promoting bacteria assessed. An increase in germination rate (30%), wet (55%) and dry biomass (40%) and shoot length (10%) were observed compared to bulk controls for all soil types.

Rose Alani (University of Lagos) spoke on *Concentrations profiles and exposure risks of atmospheric polycyclic aromatic hydrocarbons (PAHs) in Lagos, Nigeria,* a study into spatial and temporal variation in PAHs in the air, and possible exposure risks. The results ranged from residential levels of 28.82 ng m⁻³ to industrial levels of 111.93 ng m⁻³. A seasonal industrial trend was observed, with highest values in the dry season.

Saer Samanipour (University of Amsterdam) presented *A novel high-resolution mass spectrometry toolbox for unravelling the chemical exposome,* outlining a collection of open-source tools to improve and simplify non-target analysis workflows. These tools were tested on complex environmental samples including WWTP influent and sludge and were found to outperform commonly used methodologies.

Rachel Schwartz-Narbonne (Newcastle University) discussed *Detection of methanotrophic bacteria in peatlands through a novel high temperature gas chromatographic analysis method for bacteriohopanepoly-ols.* Bacteriohopanetetrol is produced by an aerobic peatland methanotoph. Its concentrations were analysed to identify that *M. palustris* may have a significant role in methane fixing and storage in peatlands.

Rebecca Rae (University of Edinburgh) delivered *Re*mediation of hexavalent chromium and selenium using

Saer Samanipour presented a novel high-resolution mass spectrometry toolbox for unravelling the chemical exposome the mineral ettringite. She discussed the sequestration of hexavalent chromium and selenium anions from wastewater through incorporation into the column material ettringite. A competitive mineral phase was also identified. Next steps include the introduction of competitive ions and recy-

cling metals via ettringite decomposition at low pH.

Phillip Colyer (University of Portsmouth) discussed *A chemical and ecological assessment into elemental loading from Ford Crossing in Ashdown Forest, Sussex, United Kingdom.* Biomonitoring and chemical analyses assessed harmful contaminants from road surface and vehicular run-off into waterways. Chromium, lead and zinc were elevated at one sample site. Elevation of zinc and magnesium were observed following rain, demonstrating waterway sensitivity.

Preston Akenga (University of Plymouth) spoke on *Uptake of antiviral pharmaceutical compounds in lettuce.* Reclaimed wastewater and bio-solids are commonly used as agricultural soil amendments. Four antiviral active pharmaceutical ingredients were identified, with concentrations up to 3450 ng g_1 (dry). Uptake

was higher than environmentally significant exposure levels and was affected by the hydrophobicity, pH and concentration in the exposure solution.

Peng Zhang (University of Birmingham) discussed *Nanomaterial transformation and phytotoxicity: Implications for food safety and application in agriculture.* Two studies investigated plant-species dependent transformation of CeO_2 nanoparticles and the phytotoxicity and transformation of graphene nanoparticles in rice plants.

Philippa Kearney (University of Bath) presented *Removal of endocrine disruptor bisphenol A from water*. She addressed the need for eco-friendly management, proposing an electro-chemical oxidative polymerisation method, with proven concept and optimised electrode surface treatment. An extraction and fluorescence based quantitative analysis method was developed as a cheap, rapid method for quantification in ocean samples.

Olumide Emmanuel Akinrinade (University of Birmingham) delivered review on *Status of flame retardants, polychlorinated biphenyls, and polycyclic aromatic hydrocarbons in air and indoor dust in Africa.* The focus was on trends of persistent organic pollutants (POPs). The primary source of the principle POPs in Africa are obsolete electronics and imported waste treatment.

Paschal Iniaghe (University of Africa) presented Concentrations *and human health risk assessment of polychlorinated biphenyls (PCBs) in canned sardines available in the Nigerian Market.* The concentrations across 15 brands were up to 926 ng kg⁻¹. Adult exposure was quantified up to 232 ng kg⁻¹ bw day⁻¹. Both carcinogenic and non-carcinogenic risks were identified associated with human consumption of these sardines.

Neville Llewellyn (Thermo Fisher Scientific) discussed *The first global reconnaissance of organic pollutants in tap water.* This involved non-target monitoring of 69 sites in 51 countries globally, representing the entire socio-economic spectrum. 1 mL samples were assessed via Q Exactive Orbitrap mass spectrometry. Contamination, including illicit drug compounds were more prevalent in developed locations. DEET was wide-spread, but high in sub-Saharan Africa.

Nina J. Schleicher (Imperial College London) spoke on *Bioavailability of trace metals in atmospheric particulate matter.* The study investigated four particle fractions in air from Beijing. Zinc, cadmium, manganese and arsenic were detectable at high concentrations in the very mobile fraction and lead and copper in the mobile fraction. Toxic elements originate primarily from anthropogenic sources.

Miguel A. Gomez-Gonzalez (Imperial College London) delivered *Intermediate speciation changes and spatially resolved transformation of ZnO nanomaterials with-in wastewater environments,* where he reviewed a new method based on *in situ* X-ray fluorescence microscopy for observing real-time dissolution and morphological and chemical evolution of ZnO nanorods with 1-3 hour incubation times in influent water and primary sludge form WWTPs. After only an hour in influent water, ZnO nanorods were completely transformed to insoluble zinc sulphide (ZnS).

Moses Ogbaje (University of Kentucky) discussed *Production and application of activated carbon sourced from agricultural wastes for water treatment.* Results showed significant but varied removal of copper (4.64-98.7 %), lead (33.3-100 %), and other metals. Activated carbon made from almond fruit had higher removal of copper, zinc and magnesium than activated carbon made from African star apple shells and snail shells.

Symiah Barnett (Aston University) introduced *The identification of microplastics using density analysis* (**page 25**), which used affordable, accessible density analysis methods to identify microplastic polymer types. The method used only water, sucrose and ethanol to distinguish eight types of microplastics by their densities. A precise solution preparation protocol was developed. Different types of microplastics float or sink in the different solutions, allowing their identification.

Theodore Dibble (SUNY College of Environmental Science and Forestry) delivered *Recent advances in understanding atmospheric mercury redox chemistry.* Mercury (Hg) is emitted to the atmosphere mainly as volatile elemental Hg(0). Oxidation to water-soluble Hg (II) plays a major role in Hg deposition to ecosystems. Atomic bromine (Br) of marine organobromine origin is the primary atmospheric Hg(0) oxidant, and then a second-stage HgBr oxidation occurs through NO₂ and HO₂ mediated radical chemistry. Full details at: www.atmos-chem-phys.net/17/6353/2017/

Vajira Perera (Sri Lanka's Tertiary and Vocational Education Commission) discussed *Development of audit criteria for water safety plan*, a brief overview of the WHO Water Safety Plan (WSP) criteria, including the deliberation and decision-making process, detailed hazard identification and risk assessment, routine monitoring, drinking water quality audits, and routine and emergency management procedures.

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Review

ClairCity webinars: engaging citizen scientists in air quality monitoring and improvement

Jeremy Thomas (Abingdon School, jeremy.thomas@abingdon.org.uk)

2020) aiming to encourage citizens and local authorities in six European countries to work together to improve air quality. Sixteen partner organisations were involved in the project, including six cities with different air pollution issues: Amsterdam (The Netherlands), Bristol (UK), Aveiro (Portugal), Liguria (Italy), Ljubljana (Slovenia), and Sosnowiec (Poland). A series of webinars in the summer of 2020 presented the outcomes of the project, especially the successful development of citizen science activities to address urban air pollution.

The project (1) was designed to give a behavioural focus to the problem of poor air quality in the cities and regions involved, rather than a technical emphasis. This meant asking questions such as what behaviours lead to the most polluting activities and why people choose to undertake them, rather than addressing vehicle numbers, fuel types and industrial activities. In this way, the project empowered individual citizens to have an impact on improving air quality in their communities by providing information on how much pollution was due to their own actions and choices. This was then coupled with modelled scenarios to predict the potential effects of altering their behaviours. A key element of the most successful projects, in Bristol and Amsterdam, was early and continuous engagement with local planners and legislators so that citizens' voices were heard, and practical, effective solutions could be negotiated.

Researchers aimed to involve citizens in decision making by addressing questions such as why people use cars for daily activities rather than other methods of transportation, what contribution these activities make to pollutant levels, and what barriers there are to behavioural change. A surprising finding was that, at least in Bristol, 40% of the relative distance contribution of car use was for leisure purposes, with commuting only coming second at 20%. Other contributions came from journeys

ClairCity was a four-year project (2016- related to shopping, business, errands, caring, and education. Citizens were next asked for ideas on what behaviours they would like to change and what would be needed to facilitate these changes. Ideas such as banning polluting vehicles, more cycle routes, and support for poorer citizens were discussed with policymakers, and changes from the 2016 baseline pollution were modelled in the study locations for each scenario. Model results were presented in terms of the effects of reducing car use for each of the separate journey types on levels of individual pollutants such as NO_x and particulate matter. In this way, citizens and policymakers could easily compare how modification of individual behaviours would make an impact. Example results for scenarios modelled in Bristol are shown in Figure 1.

> Awareness of the project was raised through various means including specially organised events, participation in existing events such as festivals, video making for older people, school lessons, online games and apps. Workshops were held to bring citizens together with policymakers and stakeholders (e.g. local industries). The Delphi method (2) was used to promote discussion at these workshops, with participants responding anonymously to questions posed in advance and the responses being discussed by the group at the meetings.

> Various engagement and social media strategies were adopted, but direct engagement through Delphi surveys was most successful in reaching those not voluntarily interested in air pollution and environmental topics. This involved physically visiting target communities with paper questionnaires, approaching people in the street, attending community events, or visiting venues such as health and community centres. Church services were a particularly good way to reach communities in Sosnowiec. Once community groups had been identified and recruited to the project, handing responsibility to them for data gathering was found to be very successful in maintaining engagement.

> Evaluation of the project was presented in a summary report (<u>http://www.claircity.eu/reports/</u>) showing that the Delphi workshops, the online game and social media coverage led to the best engagement return. The workshops led to the largest increases in understanding air pollution issues, whilst the online game and workshops both led to the largest increase in those intending to act



Road transport NOx and PM10 emissions scenarios by motive

Figure 1. From ClairCity Website (permission given).

pants enjoyed the most were the Delphi workshops and the online game, whereas the app was the least liked activity. Overall, 74% of participants in *ClairCity* projects said they would make a change to their lives in order to improve air quality. Evaluation statistics showed that enjoyment of the activity was most clearly correlated with increased understanding and likelihood of behavioural change to improve air quality.

The impact of the project on air quality will not be immediate, but it has pointed the way towards more successful ways to elicit behavioural change from individuals and to encourage local policymakers to engage their citizens in decision making. Results showed willingness by citizens to change, and a wish for greater policy ambition and speed of implementation. Quoting directly from the *ClairCity* website (1):

For instance, citizens who drive today largely want to drive less in the future and choose more sustainable alternatives for their commuting, shopping and leisure trips - across all cities and regions. Many want to choose renewable fuels in the future also, although cost is a big barrier for some cities across Europe. In some cities, a lack of awareness on certain sources of air pollutants, in particular wood burners, may be a limiting factor to citizens' ambition – Or, alternatively, citizens may not feel able to challenge authorities to do something about these issues and therefore choose not to raise them. All in all, the willingness was there, but more often than not barriers existed to prevent change from happening sooner. When local citizens' top policies were presented to

as a result of participation. The activities that partici- policymakers in their city or region, many agreed with their level of ambition, although in some instances they were slowed down, largely as a result of cost. As always with politics, a lot of negotiation and compromise is involved, often bound tightly by purse strings. However, as has been shown in Amsterdam, sometimes you can get a situation where the local government is so ambitious that its citizens are rushing to keep up. (http:// www.claircity.eu/2020/07/14/citizens-at-the-centre/)

Webinars

The four webinars are available on the project's YouTube channel (3). Each session lasts approximately one hour. The topics are:

- 1. Citizen Engagement on Air Quality and Climate Change
- 2. Seeing Citizens' Behaviour in Emissions, Air Quality & Health Modelling
- 3. Citizens in Clean Air Decision Making - Lesson for Policy
- 4. Citizens Engaging Policymakers on Air Quality and **Climate Change**

- 1. ClairCity: http://www.claircity.eu/
- 2. Dalkey, Norman; Helmer, Olaf (1963). Management *Science.* **9** (3): 458–467. doi:10.1287/mnsc.9.3.458.)
- 3. ClairCity Youtube channel https:// www.youtube.com/channel/ UChm5EPiOyBCfpjnVqhdRyKA

Meeting Report

Rethinking behaviour change at Communicate 2020

"The public conflate broader

environmental issues and cli-

mate change."

Rowena Fletcher-Wood (Freelance Science Communicator, rowena.fletcherwood@gmail.com)

Rethinking behaviour change was just one session that ran during the two-day Communicate 2020 desktop conference on 26th and 27th November organised by the Natural History Consortium. The session concentrated on the psychology of climate action, and emphasised the value of integrating professional identity with climate advocacy to drive "agency".

The session featured speaker Dr Kris De Meyer, King's College London, and was chaired by Ruth Larbey, University of the West of England.

Dr De Meyer began by discussing the value-action gap between environmental attitudes and actions. His survey findings showed that "powerless" was the word people most often associated with their feelings towards climate and environmental change; when asked what they were doing to mitigate their concerns, 98% provided consum-

er-based answers, largely connected with recycling and minimising nonessential plastic packaging. This surprisingly high result is demonstrable of the impact of consumerism on our everyday lives, driving us to think only in anti-consumerism terms when we evaluate our poten-

tial for climate action. Unsurprisingly, the two are linked: whilst a person who has always owned a car cannot see domestic plastic waste management has only a very limited environmental impact, leading to feelings of impotence. Further, the survey demonstrated that the public conflate broader environmental issues and climate change. As professionals in environmental science, this highlights an area for improved communication.

To do this, we need to reframe climate advocacy. More research or statistics will not help - the audience are convinced. Nor will more militancy be more persuasive: although counterintuitive, language of crisis actually distances most people and enhances feelings of powerlessness. However, so long as climate advocacy



remains extrinsic to identity, the barriers to change seem unsurmountable. So how do we inspire intrinsic motivation?

Dr De Meyer brought the focus onto community and, especially, professional identities. Many lack confidence in these identities because it is not immediately obvious how their identity as a parent, sportsperson, or businessperson links to "climate agency". However, these are roles in which we have more influence and can stimulate greater actions than avoiding plastic straws. As a result of work at King's College London, new conversations are

> now being developed to help guide people into recognising the useful actions they could take professionally to advocate for the environment.

> Borrowing from social psychology, Dr De Meyer advocated for incremental steps and 'self persuasion'. For example,

how they could do without, a person who has never owned one cannot see why they would. By taking a first "climate action" such as walking to work, we gradually convince ourselves we could do a little more and invest further. After a period of time and effort, this investment comes intrinsic to identity. When asked, most audience members identified their first climate action as becoming a vegetarian. This is an excellent example of intrinsic motivation because vegetarianism is identity-based.

These findings link well to those by *ClairCity* who examined public motivations to improve air quality, and which is reviewed by Jeremy Thomas on page 15.

Meeting Report

RSC Environmental Science desktop seminars

John Collins (Environment Agency, john.collins@environment-

The Royal Society of Chemistry's suite of ing organic precursors such as fructose to certain bacte-Environmental Science journals has initiated a new series of desktop seminars. cles, to create nanocomposites with useful properties At a time when travel and physical meetings are off most people's agendas, they represent a welcome opportunity to share new knowledge and achieve some continuous professional development in a forum available to a wide audience: the opportunity was seized by attendees nology in the green nanotechnology sustainability arena. from over 50 countries.

The RSC *Environmental Science* series currently has four titles: Environmental Science: Nano; Environmental Science: Water, Environmental Science: Atmospheres, and Environmental Science: Water Research and Technology

Environmental Science: Processes and Impacts. The journals aim for timely publication of new research through fast turnaround from submission to publication. The desktop seminars reflected the four interest areas.

The series was opened by Professor Peter Vikesland, Professor of Civil and Environmental Engineering at Virginia Tech, USA, and co-director of the Virginia Tech Sustainable Nanotechnology Center (VTSuN).

He is also editor-in-chief of *Environmental Science: Nano*. surrounded by just a protein capsid) or enveloped (with His talk focussed on the implications and applications of an additional lipid bilayer). Professor Wiggington renanotechnology for the environment. Vikesland started with a historical perspective on the susceptible to free chlorine inactivation than a model non implications and applications of nanotechnology over the -enveloped virus, "MS2". The inactivation mechanism of last 15+ years.

The lecture outlined a number of case studies, the first of which described how work to understand the toxicity of This difference in toxicity was attributed to differences in wastewater solids than non-enveloped viruses. the production of reactive oxygen species. This understanding led in turn led to the development of antiviral Finally, Professor Wiggington described work to develop and antibacterial applications. Another example was the models for deactivation rates of single-strand RNA virus-

ria creates bacterial cellulose. This nanocellulose can be mixed with guest nanomaterials, such as gold nanoparti-(e.g. availability as a hydrogel, and being reversibly adherent). The nanocomposites are used to enable reversible pollutant detection by Surface Enhanced Raman Spectroscopy and to produce photothermally active membranes for water treatment.

Professor Vikesland ended by proposing a single cycle perspective of applications and implications of nanotech-

The second seminar in the series, How virus structure and chemistry impacts environmental fate, was presented by Dr Krista Wiggington, Associate Professor of Environmental Engineering at the University of Michigan and

Professor Wiggington described how virus models with different characteristics are used to understand virus fate in the environment and develop new detection methods

Associate Editor. Professor Wiggington described how virus models with different characteristics are used to understand virus fate in the environment and develop new detection methods. She provided an overview of virus characteristics: they are small (e.g. 23-40 nm for norovirus and so too small for filtration), have different types of genomes (double or single stranded, DNA or RNA), and are nonenveloped (with a genome

Professor vealed that a model enveloped virus "Phi6", was more the enveloped virus with free chlorine in Phi6 was likely protein-mediated, while that of MS2 was likely genomemediated. Professor Wiggington examined the partitioning of model enveloped viruses in untreated wastewater C_{ω} fullerenes led to the finding that toxicity was signifi- compared with non-enveloped viruses, and found that cantly reduced when the bucky balls were hydroxylated. the former partitioned to a greater extent with

development of nanocellulose as a sensor platform. Feed- es and double-strand DNA viruses under UV254 light.

The model was able to predict the experimentally ob- ence between sunlight energy absorbed by the earth and strand RNA virus.

served rate for an untested subject virus within 5% and energy radiated back into space. Dry deposition is the showed coronaviruses to be highly susceptible to UV254 strongest individual source of uncertainty. Professor - more than double the next most susceptible single- Farmer described particle dry deposition as being made up of four main processes: gravity, impaction, and inter-

The third talk was from Carnegie Mellon University's Professor Neil Donahue on his collaborative work using the proton synchrotron at CERN to study the chemistry and physics of the atmosphere. The work, presented from the CLOUD consortium (https://home.cern/science/ experiments/cloud), was motivated by an interest in the cooling effects that particles such as sulfur and clouds have on the Earth's climate, i.e. in opposition to greenhouse gases like CO2. The impact of this cooling effect is more uncertain than warming. Professor Donahue's

"Particles in the air are the strongest contributors to uncertainty in radiative forcing estimates, that is, the difference between sunlight energy absorbed by the earth and energy radiated back into space. Dry deposition is the strongest individual source of uncertainty. " ception (being carried round and attaching to surfaces) for larger particles, and Brownian diffusion for smaller sub-micron particles. Size of particles drives atmospheric longevity. The lifetime of smaller particles exceeds that of larger particles. Studies by her team have shown that dry deposition influences the lifetime of particles, and that widely used parameterisations poorly capture the sizedependence of observations.

Current models overestimate cooling effects over

and physics behind particle growth and composition. A derestimate indirect cooling effects. She recommended particularly exciting example was the well-studied particle formation system of SO2 and NH3. Professor Donahue used the CLOUD chamber to observe how this process shows a stepwise increase in particle formation rate when other species (NO₂, HNO₃) are present, providing insights into particle formation routes in wintertime pollution events in cities (such as Beijing) and the importance of nitrate in contributing to health-threatening particle concentrations.

This seminar was sponsored by the RSC's new openaccess Environmental Science: Atmospheres. Attendees were given an overview of the new journal and its transparent format, including options to concurrently publish peer-reviews alongside the accepted manuscript.

The final lecture was given by **Professor Delphine Farmer**. Her talk. Masters of their fate: Revisiting atmospheric particle deposition and lifetime, was sponsored by Environmental Science: Processes and Impacts. It examined 2. how particles in the atmosphere interact with and are taken up by different topographical surfaces such as forests and grassland, as well as how those processes impact on atmospheric longevity, and consequently on climate and air quality. The means by which particles are removed from the atmosphere are via wet and dry deposition and Professor Farmer described her work looking at dry deposition.

Particles in the air are the strongest contributors to uncertainty in radiative forcing estimates, that is, the differ-

work explored the atmospherically-relevant chemistry land from direct radiative effects and substantially unmodel revision.

Summary

This desktop series provided an opportunity for the RSC to showcase its relatively new series of Environmental Science journals, researchers to publicise their work to a wide audience, whilst the range of themes examined in the presentations and the short, on-line format has enabled very many attendees to deepen their understanding, or investigate a new area of knowledge. It has been a welcome initiative.

- 1. Environmental Science: Nano (https://www.rsc.org/ journals-books-databases/about-journals/ environmental-science-nano/)
- Environmental Science: Water Research and Technology Associate Editor (https://www.rsc.org/journalsbooks-databases/about-journals/environmentalscience-water-research-technology/)
- 3. Environmental Science: Atmospheres (https:// www.rsc.org/journals-books-databases/aboutjournals/environmental-science-atmospheres/)
- 4 Environmental Science: Processes and Impacts (https://www.rsc.org/journals-books-databases/ about-journals/environmental-science-processes-<u>impacts/</u>)

Meeting report

Ideas online: Outreach from home

Rowena Fletcher-Wood (Freelance, rowena.fletcherwood@gmail.com)

In October 2020, the IF Oxford ideas fes- tions probe observational skills (for example, "What are tival (1) went online. To maximise oppor- some things you may observe when dry ice is added to tunities for participation, the festival, which usually spans ten days in Oxford, ticipants found the observation skills most challenging, was transformed into a month-long online and highlights misconceptions, such as the equivocation celebration of science, featuring a digital 'explorazone', on-demand events in the auditorium, and pre-recorded videos and resources. It was a novel and ambitious format. The ECG's "Blue Skies Science" booth (Figure 1) was resourced by eight volunteers.

It is impossible to know from afar how popular the events were - without a glimpse round a busy auditorium, a number count, or a flurry of activity that crashes the platform - but it was quiet in the live chatroom on Saturday 17th October. This is the day that, had the event been live, volunteers would have staffed stalls in Oxford to engage with the public, play with air quality monitors, and talk passionately about environmental science. Instead, we sat at home, hoping for questions.

Although a lot of preparation goes into any public engagement, IF Oxford was an extreme: between us, the team wrote, produced, edited and publicised nine videos on topics from particulate matter to microplastics to the iron content of rivers (2). This was a time-consuming activity. At the time of writing, the videos have received ~100 views on YouTube, and are accessible online (3).

Based on the videos, we also hosted a quiz (4). The ques-

ocean water and pH indicator?") and encourage learning chemical names and acronyms. Results showed that parof carbon dioxide gas and steam.

In our "How To"s, we have published resources for outreach providers and teachers, both in the *Bulletin* and online (5). However, with recent demand for resources parents can use with children at home, we also created activity sheets for participants to take home and try later. These will be appearing on our website and in our Bulle*tins* in the near future (6).

Resources

- 1. To offer Pay What Your Decide support or find out more about the festival, visit <u>https://if-oxford.com/</u> events/
- 2. To find and use our resources, visit https://if-oxfordexplorazone.vfairs.com/
- 3. To watch our videos now that the festival is over, visit https://www.youtube.com/playlist? list=PLEcpvYrIhPMYH25hcBY5oNVBo1qwi1A w
- 4. To answer our quiz, visit <u>https://docs.google.com/</u> forms/d/
- e/1FAIpQLSeG1hbWTnChjSazJl hHNHOs4dVOc6KQd 585lzXvAgPAY mt0/viewform?usp=sf link
- To view our resources for outreach providers and teachers, visit <u>https://www.envchemgroup.com/</u> resources.html
- 6. Activity sheets for children will be coming soon: Filter Funnel Engineering appears on page 21.



Figure 1. The EGG booth in the IF Oxford Explorazone Exhibit Hall.

Activity sheet

Filter Funnel Engineering

Design and test your own filtration materials to clean a sample of dirty water. Compare your work to clean and dirty samples, just like environmental scientists do.

Filtering water to make it clean enough for drinking is You'll need important work for environmental chemists. Good filters must remove particulate matter (visible bits of dirt), discolouration (dissolved materials) and even some ty cup invisible contaminants, like bacteria. Sometimes one filter just won't do, and several materials have to be used in series.

Large plastic bottle, scissors, clean and dirty water, emp-



Instructions

- 1. Cut the top \sim 5 cm off the plastic bottle and remove the lid to make a filter funnel.
- 2. Balance your filter funnel in an empty cup.
- 3. Stuff with a filter material (e.g. Cotton wool balls,).
- 4. Pour in the dirty water, collecting the filtered water in the cup below, saving a little dirty water for comparison.
- 5. Compare your filtered water to your original dirty water and some clean tap water.
- 6. Please don't drink the filtered water. It may still contain invisible contaminants!

Challenge

Experiment with different materials in different orders to design your own filter. How clean can you get the water?

Try

Cotton wool balls, baking paper, cloths, sponges ... and anything else you can think of!

Article

Mine wastes: Environmental impacts and resource potential

Karen Hudson-Edwards (Exeter University, k.hudson-edwards@exeter.ac.uk)

looked at your mobile phone, used a computer, driven your car, or used electricity. Perhaps without realising it, you have made use of mined materials such as metals, industrial minerals or energy resources. Mining has been carried out since prehistory, as humans have needed, and still need, these resources to make tools, buildings, machinery, infra- Liquid mine wastes include processing compounds that structure, artworks and other goods. Mining also provides jobs, contributes to GDP, supports cultural development and provides scientific knowledge. Mining is a global activity: Many countries currently support an industry and gain economic benefit from it, and even countries who no longer have a mining industry have toxic (3). The toxicity arises because the waters, like had one in the past.

Within the last hour, you may have cur in gaseous, solid and liquid form. Gaseous wastes include compounds produced during smelting or other processing, such as sulfur dioxide. Solid mine wastes include waste rock, tailings, slag, metallurgical materials, and contaminated river sediments. Most commonly found are tailings, which are fine-grained mixtures of crushed rock and processing fluids produced in mills, washeries, or concentrators that remain after the extracted ores are processed (2). Tailings are commonly stored as slurries in tailings storage facilities also known as tailings dams.

> are not reused, and waters that are generated from the reaction of solid mine wastes with meteoric (precipitated) waters. The latter, called 'drainage', are classified into three major types according to their pH. The most common and deleterious of these is 'acid mine drainage' (AMD) (Figure 1a), which exhibits pH values from -3.5 to 5 (3). The pH of circum-neutral mine drainage (CMD) varies between 6 and 8, and that of basic mine drainage (BMD) varies between 9 and 12. AMD, CMD and BMD can be radioactive, corrosive and highly solid mine wastes described above, can contain elevated concentrations of metals and metalloids that, if ingested

Some of the materials extracted through mining, including industrial minerals like gypsum, are fully utilised. Others, like metals, only form a small proportion of the material extracted. This means that a large percentage of the extracted materials are wastes. Because most high-grade ores have now been exploited through mil-

lennia of mining, contemporary ores are much lower neutralisation that takes place for AMD and BMD. For grade. As a result, we are now producing more waste from mining than ever before. But what is this waste? Should we be concerned about it? And can we make use of it?

What are mine wastes?

Mine wastes are defined as "materials originating, accumulating and present at mine sites, which are unwanted and have no current economic value" (1). They can oc-

"Mine wastes are defined as "materials originating, accumulating and present at mine sites, which are unwanted and have no current economic value"."

or inhaled by organisms, can cause lethal or sub-lethal effects. Examples are shown in Table 1. Metal and metalloid concentrations of AMD waters are generally higher than those of NMD or BMD waters, although BMD waters often contain high concentrations of metalloids that form anions (e.g. As). Concentrations are variable, depending on the ore mineralogy and degree of

solid mine wastes such as tailings, metal and metalloid concentrations also vary depending on the geology of the ore deposit, and type of economic commodity that has been extracted. Tailings can either have elevated concentrations of a suite of metals and metalloids (e.g. Potosí, Bolivia) or one or two metals (e.g. King Mine, California).

Site	Iron Moun- tain, Cali- fornia ¹	Wheal Jane, Cornwall, UK ²	Angoran, Iran (Sample W4) ³	Zhong- tiaoshan, China ⁴	Site	Potosí, Bolivia ⁵	Boliden, Sweden ⁶	King Mine, Califor- nia ⁷
Туре	AMD	AMD	NMD	BMD	Туре	Tailings	Tailings	Tailings
рН	-2.5	3.5	7.5	9.38				
SO4 ²⁻	760000	1390	2294	1582	S (%)	19.8	17.8	0.08
As/mgL ⁻¹	n.d.	2.1	0.035	2.41	As/mgkg ⁻¹	6960	2960	3.0
Cd/mgL ⁻¹	211	n.d.	0.00006	0.017	Cd/mgkg ⁻¹	62.1	16.6	0.1
Cu/mgL ⁻¹	4760	<0.008	0.026	0.004	Cu/mgkg-1	502	640	15.4
					Hg/mgkg ⁻¹	n.d.	8.4	374
Pb/mgL ⁻¹	11.9	n.d.	0.123	0.06	Pb/mgkg ⁻¹	2180	1850	2.5
Zn/mgL ⁻¹	23,500	125	n.d.	0.012	Zn/mgkg ⁻¹	26600	5290	48

Table 1. Selected examples of sulfate, metal and metalloid concentrations of AMD, NMD and BMD, and mine tailings (3-9).

Environmental impacts of mine wastes

Legacy and contemporary mine wastes have had and still Significant global effort is being made to reduce the negahave negative impacts on water and soil quality, and eco- tive impacts of mine wastes. Part of this effort is directed system and human health (2, 10). These impacts general- towards viewing mine wastes as resources. This includes ly arise from the elevated con-

centrations of potentially toxic metals and metalloids (e.g. **Table 1**)that contaminate waters and soils, and cause negative health impacts such as poisoning and cancers (11). Other negative impacts include increased sedimentation of rivers and estuaries due to large inputs of wastes to these environments (12), and tailings dam failures (2). The

latter are catastrophic events in which the embankment laboratories for studying extreme conditions of pH, metal and ecosystems and, in some cases, death. Recent analysis has suggested that the severity of tailings dam failures is increasing as mining of lower grade deposits generates higher amounts of tailings, and larger dams are being built to accommodate them (13).

A new frontier: mine wastes as resources

"[Mine wastes] are unparalleled natural laboratories for studying extreme conditions."

recovering economic metals from tailings (14) and AMD (15), using wastes to manufacture products such as bricks, cement, floor tiles and pigments (16), sequestering CO₂ in ultramafic wastes (high alkaline igneous rocks (17)), and adding wastes to soils as amendments (16).

Mine wastes have other value. They are unparalleled natural

walls fail, and large volumes of tailings solids and inter- and metalloid concentrations and bacteria and other stitial water are released suddenly into river catchments, organisms that are adapted to these. Metallophyte plants causing erosion, deposition, destruction of infrastructure have developed on mine wastes globally; these stabilise the wastes and, if they sequester metals and metalloids in their roots, prevent further accumulation up the food chain by grazers on their roots. The 80 km long AMD Río Tinto, SW Spain, is used as an analogue site for Martian research (18).



Figure 1. Examples of mine wastes. (a) Acid mine drainage and soluble sulfate salts, Cyprus; (b) Leadbearing solid mine waste, Yorkshire Dales, UK.

Research gaps

Over the past two decades, we have developed a good basic understanding of the environmental impacts and resource potential of mine wastes. There is more to do to better understand the speciation of metals and metalloids, how they are taken up in minerals and biota, the role of microorganisms in their release and storage in the environment, their global health impacts and the ways in which we can recycle, reuse and remediate them. We are now mining 'green technology', or 'critical raw materials', in much greater quantities than before to meet the demand for a low carbon economy, and there is work to do to better understand and manage the wastes produced.

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ECG Environmental Briefs No. 23

ECGEB No 23

The identification of microplastics using density analysis

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gos Institute of Marine Conservation aims to identify and quantify microplastics in the environment to investigate the main source of influx of microplastics into the Aegean Sea. This necessitated finding an affordable and accessible way of identifying the types of polymer present in the marine environment.

Microplastics

Across the world more than 320 million tons of plastic are produced each year, and recent studies show between 5 to 13 million tons of that plastic are floating in the ocean (1). To date, plastic has been found in 267 species (2) and notoriously causes harm to marine animals, mostly through entanglement, strangulation and ingestion (3). Plastics found in the ocean undergo fragmentation driven by photochemical, physical, and biological degradation to form microplastics (4). Microplastics are particularly problematic since they are often ingested by marine biota. Upon ingestion of plastics the contaminants imbedded in plastic are transferred to organisms (5). The polymer type affects the ease with which the contaminants are transferred from plastic to organisms (6). Thus, the identification of microplastic is important. In addition to this the ability to identify its polymer type gives some idea of the microplastic's source.

Techniques for identifying polymers

There are numerous techniques for identifying polymers. These include Fourier-Transform Infrared (FTIR) spectroscopy, Raman spectroscopy, Near-Infrared (NIR) spectroscopy, Short-Wavelength Infrared (SWIR) spectroscopy, Nuclear Magnetic Resonance (NMR) spectroscopy, scanning electron microscopy and Pyrolysis-Gas Chromatography-Mass Spectrometry (Pyr-GC-MS) (7). However, these techniques are not practical in remote field locations, since they require fixed, expensive equipment costs also makes them financially impractical for NGOs and small institutes.

Density analysis

Separating and identifying plastics based on their density offers a cost-effective and time-efficient field alternative.

The Microplastic team at the Archipela- they will sink or float depending on the density of the solution they are in. This technique is not novel since a considerable amount of literature has been published on



Figure 1. Test tube demonstrating density analysis of polystyrene, polypropylene, polyethylene and polyvinvl chloride

the separation and identification of plastics using their density. Morét-Ferguson et al placed a piece of plastic in distilled water and if the plastic sank, concentrated CaCl₂ or $SrCl_2$ was added until the plastic was neutrally buoyant. However, if the plastic floated, ethanol was added until the plastic was neutrally buoyant (8). The main drawback with this method is the continuous addition of a solution until the plastic became buoyant is time consuming. Similarly, in order to identify unknown plastics, Kolb and Kolb created solutions with varying densities and then recorded which plastics floated or sank (9). Unfortunately, they used hazardous solutions to carry out separation. Syakti extracted microplastics from mediums based on the principle that different polymers have different densities. This method used density to separate the microplastic, not to identify the microplastics (10). Nevertheless, this research alongside all the literature mentioned above demonstrates that density analysis can Since different types of plastics have different densities, be used to separate and identify the plastics, and this technique could be used for identification in environmental analysis.

Density analysis to identify microplastic in environment

At Archipelagos Institute of Marine Conservation research was carried out to identify eight types of microplastics based on their densities which involved only the 2. Teuten, E., Rowland, S., Galloway, T. and Thompson, R. use of water, sucrose and ethanol. The plastics used were polyethylene terephthalate, high density polyethylene, polyvinyl chloride, low density polyethylene, polypropylene, polystyrene, expanded polystyrene and polyamide. Following precise protocols, eight solutions of known densities were prepared, and the microplastics were placed in these solutions contained in different test tubes. Since different types of plastics have different densities, they sink or float depending on the solution they are in. The buoyancy of the microplastics in the solutions is observed using a magnifying glass or microscope, and this is used to identify the microplastics' polymer type. This technique was verified in the field with microplastics recovered from the Aegean Sea. The plastic -team took plastic that was identifiable by the recycle symbols from the environment, filtered them, treated them, and then converted them into microplastics (< 5mm) using a scalpel The plastic samples were placed in containers labelled A-H, and as the type of plastic was unknown to us, the method was validated by a blind test. The test was carried out on three separate occasions.

Why do we need this technique?

Often NGOs and small institutes tackle plastic pollution in remote and inaccessible locations, so it is imperative that they are equipped with a technique that enables them to identify microplastics, and as a consequence combat plastic pollution. Density analysis offers a cost-effective and time-efficient alternative way of separating and identifying plastics in the field.

Conclusions and further research

This procedure offers a quick and inexpensive way of roughly identifying the main sources of microplastic pollutants in the environment when working in the field.

However, there are a few limitations that need to be considered. Firstly, only eight polymer types were investigated, whilst there are a significantly more polymers. Secondly, sampling variation was limited by testing samples collected from a single source. Hence, a wider range of sources is recommended to further develop this procedure. Also, further verification via infrared spectroscopy is something that could be done to increase verity. Finally, the same polymer can appear in microplastics with different densities. For example, polystyrene and expanded polystyrene are the same polymer, but modification during production gives the plastic very different properties and uses. In fact, modification, such as moulding and extrusion, changes its density (11). Nevertheless, this provides a good starting point for discussion and further research into inexpensive ways of identifying microplastics.

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EGC Environmental Briefs No. 24

ECGEB No 24

Surface complexation modelling: building tools to understand and predict adsorption Jay C. Bullen (Imperial College London, j.bullen16@imperial.ac.uk)

Surface complexation models (SCM) are What is a SCM? important tools for environmental chemists, allowing us to understand and predict adsorption in complex systems. This complexation reactions are modelled using equilibrium Brief introduces SCM, describes how a new modeller gets started and develops their own models, and highlights some advanced SCM applications.

The Langmuir and Freundlich adsorption isotherm models are well known; indeed, they are taught in most undergraduate chemistry courses (1). However, these models describe single-sorbate single-sorbent systems, and are only valid for the specific conditions under which the model's parameters were experimentally determined. Surface complexation models (SCM) provide a more sophisticated description of adsorption, sensitive to changes in environmental conditions including pH, ionic strength and the presence of competitor ions (2). SCMs have important applications, such as determining the mobility of toxic heavy metals and essential micronutrients in groundwater and soil (3), and understanding the performance of synthetic sorbent materials for the remediation of contaminated waters (Figure 1) (4).



Figure 1. Predicted speciation of arsenic (III) adsorbed onto a mesoporous TiO2/Fe2O3 composite. Conditions: 32.1 mg L-1 total As(III), 1 g L-1 sorbent, pH 7, 0.01 M NaCl. Surface complexation model was calculated following Bullen et al. (2020).

Surface complexation models use the analogy of solution phase metal-ligand complexation to describe the adsorption of a dissolved sorbate onto a solid surface. Surface constants and the activities of reactants M (representing the sorbate) and L (representing the functional groups of the sorbent) and the product (ML):

$K = a_{ML} / a_M a_L$

Electrostatic forces can significantly influence the extent of adsorption. For instance, the attraction between a positive iron oxide surface and negative $HAsO_{4^{2}}$ anions at neutral pH shifts the equilibrium position towards the products. Electrostatics are accounted for by modifying the intrinsic equilibrium constant with an electrostatic term, yielding an 'apparent' equilibrium constant:

 $K_{apparent} = K_{intrinsic} \cdot exp \cdot F\Delta\Psi/RT$

where ψ is the surface potential of the sorbent (V) (2).

Running the first model

Several software packages with SCM capabilities are freely available (e.g. Visual MINTEQ and PHREEQC). Both offer introductory tutorials and contain databases of the equilibrium constants needed to model many aqueous phase and surface complexation reactions.

These databases firstly define a selection of components or master species. Each component is like a Lego block: components such as AsO_4^{3-} and H^+ can be combined in different ways to yield different chemical species, including AsO43-, HAsO42-, H2AsO4-, H3AsO4, H+, and OH-. The surface hydroxyl component, >SOH, can be similarly combined to yield surface complex species such as >SOH₂⁺, >SO⁻, >SOAsO₃²⁻ and (>SO)₂HAsO₂.

The SCM also requires several physical parameters: (i) the sorbent surface area, and (ii) the site density (the number of surface functional groups per square nanometre) are needed to calculate the total adsorption capacity. Many SCMs also require (iii) a value for the capacitance of the electrical double layer (EDL). Like the equilibrium constants, these parameters can be obtained from the literature when running your first model.

After defining the SCM parameters, the user enters the pH and concentrations of the sorbent, sorbate, electrolyte



Figure 2. Development and validation of surface complexation model for the adsorption of arsenic(V) (AsO₄³⁻) onto goethite (FeOOH). Figures based upon Bullen et al. (2020)

and any competitor sorbates. Running the program calculates the speciation of the system (*e.g.* Figure 1).

When performing an experiment, the user often wants to know how one variable influences another. This is achieved using the sweep function in Visual MINTEQ and by programming loops (using Visual Basic) within PHREEQC.

Building your own model

Sometimes it is necessary to calculate SCM parameters – if the user cannot find their specific sorbate-sorbent combination in the literature, or previous models are out -of-date (*e.g.* using disproven surface complexes). SCM parameters are best calculated from experimental data using non-linear regression: an initial guess is made for each parameter, and an algorithm varies these values until the sum of squared residuals between experimental data and the model's output has reached a minimum (5). Software such as FITEQL and Visual MINTEQ offer this functionality.

However, these algorithms can only optimise a limited number of parameters per experiment and it is therefore best to develop our model in stages:

- Physical parameters must be defined. The surface area of the sorbent is best determined experimentally (BET analysis). Site densities are difficult to determine experimentally and may be estimated from adsorption data or optimised to fit the model (2).
- Surface charge is heavily controlled by the pHdependent (de)protonation of surface hydroxyls. Equilibrium constants for these reactions are normally calculated by optimising the model to fit experimental potentiometric titration data (Figure 2a).
- 3. Many sorbates form a pH-dependent variety of surface complexes. Consequently, equilibrium constants for the adsorption of our analyte are best calculated by fitting the model to experimental pH adsorption edges (**Figure 2b**).
- 4. Finally, it is important to validate the model by predicting new chemical behaviour and comparing the results with unseen experimental data. The compari-

son of SCM-predicted adsorption isotherms with experimental data is often a good way to validate the model (**Figure 2c**).

The potential of SCM

SCMs are versatile. Multi-sorbate SCMs predict competitive adsorption in complex solutions. Component additive models (CA-SCM) predict adsorption onto new composite materials as a function of their surface composition (4). SCMs are easily integrated with other models, *e.g.* Visual MINTEQ provides the databases and calculations necessary to simultaneously model (i) adsorption onto minerals, (ii) ion exchange with clay minerals, and (iii) soil organic matter complexation (6). Finally, SCMs can provide new insights into adsorption mechanisms, *e.g.* helping identify multilayer adsorption or the formation of ternary surface complexes.

If you like to learn surface complexation modelling, Visual MINTEQ and PHREEQC are good places to start:

https://vminteq.lwr.kth.se

https://www.usgs.gov/software/phreeqc-version-3

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Modelling antibiotics in the aquatic environment using fugacity concepts

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Antibiotics are a major concern due to the emergence of antimicrobial resistance (AMR). In the absence of intervention to prevent the environmental spread of AMR, this could contribute to 10 million deaths per year, making it more deadly than cancer (1). Understanding how antibiotics behave in the environment is important to predict their chemical fate once discharged into surface waters. When modelling compounds such as antibiotics in the environment, fugacity describes their ability to move between two environmental compartments, such as air and surface water (2).

In modelling, equal fugacity (escaping tendency) is expected in both phases as is the vapour pressure of the compound. The relationship between fugacity (f), Concentration (C, mol m^{-3}) and fugacity capacity (Z, mol m^{-3} Pa⁻¹) is shown below (**Eq 1**). The Z value is specific to a chemical, which is also dependent on the phase in which it is present. A compartment with a higher fugacity capacity capacity can accept a higher concentration of a given micropollutant.

C = Z x f (Eq 1)

Partition Coefficient

The partition coefficient is an extremely important parameter in fugacity calculations. There are several important partition coefficients, besides the fundamental properties of vapour pressure and aqueous solubility, which are essential for understanding chemical transfer ($\mathcal{3}$) (**Figure 1**).

"It is important to consider that ionisation may occur in antibiotic chemical structures at environmental pH values."

Fugacity modelling is defined by levels (*1, 2*, and *3*), which increase with complexity. Calculations can either use fugacity principles, or specific partition coefficients, as demonstrated in **Figure 1**.

In this article, calculations will use fugacity principles demonstrating level 1 and 2 models.



Figure 1. Illustration of the important partition coefficients that should be considered when modelling organic contaminants.

Level 1 Modelling Concepts

Level 1 assumes that the volumes of the compartments being studied are held constant, and the system is closed and in a steady state equilibrium. This means that the concentration of a contaminant in the compartment is

> uniform. With these assumptions, level 1 calculations can determine the partitioning behaviour of contaminants like antibiotics in the aquatic environment.

In order to accurately evaluate the concentrations of a contaminant such as an antibiotic using the fugacity method, Z values for each

using the fugacity method, Z values for each phase must be defined (air, water, and sediment for three compartments). From this, equilibrium concentrations can then be deduced using fugacity as a common criterion for equilibrium. Definitions of relevant Z values are presented in **Figure 2**, where, H = Henry's Constant, Koc = 0.35 K_{ow} (organic carbon partition coefficient), y_{oc} = mass fraction of organic carbon), R = molar gas constant (8.314 Pa m³ mol⁻¹ K⁻¹).

define concentrations in each phase, if the volume (V) of made that at any given instant, the different phases are in each phase is estimated (m3). The amount of chemical equilibrium with one another, unlike level 3 calculations, (M) in moles in a three-compartment system can be which are more complex, such that equilibrium is not measured using the following relationships to calculate assumed (5). fugacity.

$$M = fZ_A V_A + fZ_W V_W + fZ_S V_S$$
 (Eq 2)

$$f = M/(Z_A V_A + Z_W V_W + Z_S V_S)$$
(Eq 3)

Once the common fugacity has been calculated within the system, concentrations within each phase can be calculated using the specific Z-value, and f, using Eq 1. From



Figure 2. Relationships between fugacity, Z = values and partition coefficient, where C represents concentration in a specific phase organic contaminants.

this, the moles, and percentage of the compound in each compartment can also be deduced.

It is important to consider that ionisation may occur in antibiotic chemical structures at environmental pH values. This is because of the various acid dissociation constants (pK_a values) within an antibiotic. In order to compensate for this, the Henderson-Hasselbalch equation is used to evaluate the degree of ionisation at specific pH values (Eq 4, where A is the anion and HA is the neutral compound. When considering ionisation, it is the $Z_{\!\scriptscriptstyle \rm w}$ (water phase) value, which will be affected, since ionisation will occur in the water. Therefore, the new Z_w value will be $Z_w(I + 1)$, where I is the degree of ionisation. This is important, as most antibiotics will have some degree of ionisation within the aquatic environment. Certain antibiotics may even have two dissociation constants and form Zwitterions (4).

 $pH = pK_a + \log [A^-] / [HA]$ (Eq 4)

Level 2 Modelling Concepts

A Level 2 fugacity model describes dynamic environ-

ments, where there are presumed inflows and outflows Using these Z values for individual antibiotics, we can of chemicals within the compartment. The assumption is

> In level 2 modelling, the process of advection is considered. Advection can be thought of as transporting a chemical (such as an antibiotic) into or out of the region of interest by the flow of a supporting medium. The rate of advection (N mol h⁻¹) (Eq 5), is simply the product of the flowrate of the advecting medium (G m³ h⁻¹) and the concentration of the chemical in that medium (C mol m-³) (2).

$$N=G \times C$$
 (Eq 5)

The following equations (Eq 6, 7) show how advection can be incorporated into fugacity calculations to define concentrations in each phase, where, I = total influx of contaminant. The important point here is that the inflow and outflow concentrations are assumed to be equal. Using a common fugacity, and applying Eq 1, the concentrations in each phase can be defined.

$$I = fG_A Z_A + fG_W Z_W + fG_S Z_S$$
(Eq 6)
$$f = I/(G_A Z_A + G_W Z_W + G_S Z_S)$$
(Eq 7)

Many contaminants degrade in the environment, and therefore this must also be considered in level 2 simulations. When applying the concept of degradation, it is convenient to use a simple first order kinetic expression to define degradation (Eq 8).

$$dC/dT = -ck$$
 (Eq 8)

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Phosphate oxygen isotopes – A new tool for nutrient sources and cvcling

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challenge facing freshwater ecosystems and is closely associated with the anthropogenic enrichment of phosphorus (P) in $using \delta^{18}O_{P04}$ and goes on to show how the approach has the aquatic environment. Unlike nitrogen, phosphorus has only one stable isotope, ³¹P, of limited availability. This, in turn, has limited our understanding of phosphorus sources and hence the triggers for eutrophication in natural systems. Following recent advances in biogeochemical cycling techniques using phosphate oxygen isotopes ($\delta^{18}O_{PO4}$), these were mediation, negligible isotope exchange occurs between P_i identified as an effective tracer of phosphorus provenance and dynamics.

Eutrophication occurs when nutrients are oversupplied to freshwater bodies, causing excessive plant and algal growth, which can lead to oxygen depletion. It is well established that high human population densities and intensive agriculture cause the oversupply of P to fresh-

"The study showed two distinct isotopic signatures for drinking water could be identified."

waters, resulting in eutrophication and a variety of other problems for the environment and human society. Phos- 4. phorus inputs to catchments are usually dominated by diffuse sources related to various farming activities and geological hotspots, but in more heavily populated catch- 5. Precipitation of Ag₃PO₄. ments, point sources such as wastewater treatment plants (WWTPs) are of great importance.

The past few years have seen substantial advances in the use of phosphate ${}^{18}O/{}^{16}O$ analysis ($\delta^{18}O_{P04}$) as a way of identifying sources of phosphate and their fate and transport in the environment. Phosphate oxygen isotopes have previously been used within both the archaeological and environmental communities to determine the palae-

Eutrophication is a globally significant oclimatic conditions at the time of formation of biogenic phosphatic material, such as apatite (Ca₅(PO₄)₃(OH,F,Cl)) in fossil bones and teeth. This article outlines the theory behind source identification and biogeochemical cycling been tested and applied to various natural systems, which present different challenges.

Sources and cycling

In natural aquatic ecosystems, P is often bound strongly to 0 in the form of the dissolved inorganic phosphate ion (P_i, PO₄²⁻). The P-O bonds are resistant to inorganic hydrolysis under the typical temperature and pressure conditions found in the Earth's surface water and groundwater ecosystems. Therefore, without biological and water, hence, based on the isotopic composition, a 'source' (e.g. wastewater or fertiliser) may be identified. In contrast, enzyme-catalysed processes cleave P-0 bonds leading to kinetic or equilibrium fractionation between the isotopes of O in P_i and O in a surrounding fluid. Hence, there is a shift in the $\delta^{18} O_{P04}$ composition towards an equilibrium value as a result of biogeochemical cycling.

Extraction methods for inorganic P

There are a number of published protocols (1) for extraction of P_i via precipitation of Ag₃PO₄ for analysis by massspectrometry following thermal conversion to CO. There are commonalities across these protocols, particularly

- Concentration of P_i through co-precipitation of P_i 1. with brucite (Mg(OH)₂), following the magnesiuminduced co-precipitation (MagIC) method (2);
- 2. Redissolution of the brucite precipitate in an acid matrix:
- Removal of other potential sources of 0 using anion 3. exchange resins and/or sequential precipitations;
- Removal of cations that have the potential to interfere with Ag₃PO₄ precipitation, using a cation exchange resin;

None of these previously published protocols represented a definitive approach for all aquatic matrices (2).

Isotopic fingerprint of mains water

The 17-step extraction protocol eventually developed was initially tested on mains distribution water (3). Public water utilities in the UK and parts of Europe and North America routinely dose drinking water supplies

with phosphate to prevent pipe corrosion and the dissolution of lead. This, coupled with leakage from distribution networks, represents a significant input of phosphorus to the environment. The study (3) identified two distinct isotopic signatures for drinking water. Depending upon the source of acid used, drinking water $\delta^{18}O_{PO4}$ was isotopically distinct from a number of other phosphorus sources. As such, $\delta^{18}O_{P04}$ may be an effective a tool for identifying mains water leakage as a source of phosphate in the environment.

Wastewater treatment plants

As a response to eutrophication, discharge consents for P were introduced for WWTPs, leading to capital and operating investment in P removal through tertiary treatment and other technologies. However, WWTPs can still be a significant source of aquatic P. A comprehensive study of the $\delta^{18}O_{PO4}$ composition of effluent from WWTPs produced a wide range in delta values, reflecting in part the different treatment processes applied at each site (4). A strong positive correlation between $\delta^{18}O_{P04}$ and $\delta^{18}O_{H20}$ suggested biologically-mediated exchange between water molecules and the phosphate ions. Detailed timeseries data with different treatment technologies revealed that the $\delta^{18}O_{PO4}$ composition remained constant over a 24 hour period, even though P concentrations showed considerable diurnal variation. Studies that considered instream processing (i.e. biological turnover) of $\delta^{18}O_{PO4}$ downstream of WWTPs showed evidence for mixing of the upstream source with effluent water, but

> "The isotopic approach not only identified sources but also was able to differentiate between potentially different seasonal sources."

no evidence of biological cycling 3 km downstream. Hence, $\delta^{18}O_{PO4}$ can be an effective tool to trace P from WWTPs provided that the source of the effluent is known and samples are collected within a day.

Catchments scale sources

At the catchment scale, rivers are receptors for multiple nutrient inputs, which can vary on a seasonal basis. A study undertaken in a strongly nutrient-impacted catchment in the south east of England (5) showed marked 4. D.C. Gooddy, Appl. Geochem. 95, 139 (2018) changes in phosphate concentrations between summer 5. D.C. Gooddy, Water Res. 88, 623 (2016) and winter, with highest concentrations in the summer 6. M. Tcaci, Environ. Sci. Technol. 53, 10288 (2019) when river flow was low. In contrast, $\delta^{18}O_{P04}$ values indicated a common agricultural source in the upper reaches of the catchment, and identified wastewater effluent as the dominant P source in the lower reaches, independent



Figure 1. Schematic diagram of twist spin method (TSM) experimental setup. The inlet to the column is fixed at an angle of 30° at the base to induce spinning of the water column as it twists through the resin.

of season. Hence, the isotopic approach not only identified sources but also was able to differentiate between potentially different seasonal sources.

The next step – Lower, faster

The analytical protocols described here for determining $\delta^{18}O_{P04}$ are unable to generate reliable data for samples in which ambient P concentrations are extremely low (typically $< 2.5 \mu$ mol L⁻¹). This is because, for lower concentrations, larger volumes of water need to be processed and passed through ion exchange resins which may take in excess of a week. Above 50 - 100 L of water the ion exchange resins swell and block. To overcome this problem at low concentrations of P, a new method called the 'twist spinning mode' (TSM) has been developed (6). By using the ion exchange resin suspended in a specially designed column (Figure 1), this method can process 1000 L in 24 hours and provide accurate data down to 0.5 μ mol L⁻¹. This advancement in $\delta^{18}O_{PO4}$ may provide new and important insights into the biogeochemical phosphorus cycling.

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