EMCON

BOOK OF ABSTRACTS

International Conference on Emerging Contaminants

September 13–14, 2021

Virtual Event Hosted by University of Washington

Emcon 2021

7th International Conference on Emerging Contaminants

Virtual Event, September 13-14, 2021

On behalf of our Scientific Committee and the University of Washington, **we welcome you to Emcon 2021**, the 7th International Conference on Emerging Contaminants (https://cvent.me/7kvWG9). At Emcon 2021, we have a great technical program focused on the latest research news and discoveries concerning the environmental chemistry of emerging environmental contaminants and their management. We are all really excited about our presentations, including great keynote, platform, lightning talks, posters, and unscheduled presentations. We also hope you will find our community program just as strong, please do take time to meet and chat and say hello to attendees both known and not-known-yet. While we all wish we were available to meet in person, we welcome you in this most challenging year to a virtual version of EMCON as we all learn how to cope with science and network and community and family in a more distant and isolating world. Conferences are made by their audiences; remember that means you and your participation is critically important throughout our program, even for a virtual event. We especially encourage you to use the discussion boards and chat rooms to virtually reconnect with old colleagues and meet new friends from around the world while discussing your exciting research and ideas together as a community. While we have to give up some conference things we love in a virtual format, please do not forget that we also have available new tools if we all take the time to learn them and make them work for us together.

We also are excited to highlight many strong presentations from our young scientists, please do take some time to look at posters and unscheduled presentations from our student presenters. Please do say hello and offer some encouraging words and feedback for all of the students attending.

Our sponsors are also critically important parts of our community. Emcon 2021 is proudly sponsored by Agilent, Eurofins, SCIEX, the Washington Department of Ecology, ACS Environmental Science & Technology Letters, and the Royal Society of Chemistry. Without their financial support, we could not provide the administrative and technical support to hold this virtual conference or offer reduced or free admission for students or need-based attendees. Please do recognize their help and assistance by saying thanks and learning who they are by saying hello or visiting their virtual platforms to hear of some new capabilities, get some technical advice, or build your capacities for research and networking.

Every virtual format requires some learning and familiarization time. Please try and spend some time on the online platform before the conference; learn how to navigate and move between the sessions and question sessions and troubleshoot any issues you have. Presentations are scheduled to go live as the conference starts, although virtual networking is available throughout the conference period. Pre-recorded content will enable both synchronous and asynchronous attendance and interaction, please familiarize yourself with the technical program and schedule. We look forward to seeing you! Please email emcon2021@uw.edu if you had any questions for us. Welcome!

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Emcon 2021 Technical Agenda

with links to abstracts

Keynote Presenter
Presenter
Student Presenter
Audience Driven Event

All times listed are Pacific Daylight Time (PDT)
All talks will be prerecorded, and available asynchronously
All questions and discussions will be live, and panels of immediately previous speakers, with live and chat questions

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Acrobat Reader: Right click on the top toolbar and choose "Show all page navigation tools" **OR**
If you click on a hyperlink in the agenda or on the sidebar and then wish to return to the page you linked from (previous view), the keyboard combo on a PC is Alt + ← (arrow pointing left on your keyboard)or on a Mac ⌘ + ← (arrow pointing left on keyboard)

Monday, September 13, 2021

Networking and Opening Remarks

Times: PDT	
500-900	**Informal Mingle and Open Chat/Networking/Chat Rooms open**
900-910	**Welcome and Greeting**
	Host-Kolodziej: Welcome to ENCOM 2021
910-915	**How to use the platform**

Microplastics

915-1000	Keynote: Chelsea Rochmann, University of Toronto
	The Multi-Dimensionality of Microplastics – And How That Influences Their Fate and Effects in Aquatic Ecosystems
1000-1015	Platform 1: E. Okoffo, U. of Queensland
	Plastics contamination in archived biosolids from 1950 to 2016
1015-1030	**Questions/Discussion**
1030-1045	*Break (or Eurofins Live session)*
1045-1100	Platform 2: L. Tseng, Colgate U.
	Adsorption of contaminants of emerging concern (CECs) on large and microplastic polyvinyl chloride, polyethylene, and polystyrene
1100-1115	Platform 3: T. Toapanta, U. of Queensland
	Signal decrease of microplastic polypropylene due to simulated weathering during quantification analysis with Pyrolysis Gas Chromatography Mass Spectrometry
1115-1130	Platform 4: M. Nanny, U. Oklahoma-Norman
	Using Cell Cytometry and Raman Spectroscopy to Characterize Microplastic Particles < 300-Microns in Water Samples
1130-1145	Platform 5: S. Siddiqui, Oregon State U.
	The Internalization And Sub-Lethal Effects Of Tire Wear Micro And Nanoparticles On Two Estuarine Indicator Species
1145-1200	**Questions/Discussion**
1200-100	*Lunch Break*

Roadway Runoff

100-145	Keynote: Zhenyu Tian, Northeastern University
	Occurrence and Temporal Trends of the Coho Salmon Toxicant 6PPD-Quinone in Urban Creeks
145-200	Platform 6: J. Challis, U. of Saskatchewan
	Occurrences of tire rubber derived contaminants in cold-climate urban runoff
200-215	**Questions/Discussion**
215-230	*Break*
230-245	Platform 7: C. Rauert, U. of Queensland
	Linking occurrence of tyre road wear particles (TRWP) and tyre additive chemicals in Australian urban water cycles
245-300	Platform 8: E. Rodland, Norwegian Institute for Water Research
	Quantification of tire and road wear particles and associated road pollutants in a Norwegian tunnel system
300-315	Platform 9: R. McKane, Environmental Protection Agency
	Model analysis and visualization of 6PPD-quinone fate and transport in Longfellow Creek watershed, Seattle, USA.
315-330	**Questions/Discussion**
330-345	*Break (or Eurofins Analytical Live session)*

CEC Sources

345-400 Platform 10: J. Masoner, U.S. Geological Survey

Comparison of Organic Chemical Contributions to Receiving Waters from Discharge of Multiple Reuse Waters and Potential Concern to Aquatic Organisms and Human Health

400-415 Platform 11: L. Hubbard, U.S. Geological Survey

The first comprehensive chemical and biological characterization of wastewater from food, beverage, and feedstock processing facilities across the U.S.

415-425 **Questions/Discussion**

425-430 *Break*

Posters, Networking, and Community

Times: PDT

430-510 **Lightning Talks (5 Min Each)**

Hattaway et al.

Using spatial and temporal patterns in an urban sewershed for prioritization of nontarget features

Wang et al.

Identification and assessment of emerging contaminants in drinking water, wastewater, and surface water in Kampala, Uganda

Lenka et al.

Estimation of microplastics in drinking water: A case study of indiect potable reuse

Monaghan et al.

Condensed phase membrane introduction mass spectrometry (CP-MIMS) for direct, time-resolved analysis of 6PPD and 6PPD quinone

Nagorzanski et al.

Passive sampling behavior of electrospun nanofiber mats with embedded carbon nanotubes for emerging contaminants in water and air

Steigerwald et al.

Targeted perfluorooctanesulfonate (PFOS) removal by spent coffee biochar modified with a PFOS molecularly imprinted polymer

Sharma et al.

Characterization and optimisation of novel bacterial laccases for the degradation of aromatic organic pollutants

510-730ƀ Poster Session and Networking

Open chat rooms and networking booths

600-615 "The instrument is smoking, audience stories of doing research and what went wrong"

Do you have a story to tell? Open chat rooms and networking booths

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Tuesday, September 14

Networking

Times: PDT

500-900 Informal Posters, Hello and Networking in the EU/East Coast

Saying hello, learning the software platform, wandering around together

CECs and Food

900-945 Keynote: Benny Chefetz, Hebrew University

Pharmaceuticals and personal care products in the agriculture-food: Current knowledge and future perspective

945-1000 Platform 12: G. Lefevre, U. of Iowa

Probing Putative Transporter-Mediated Plant Uptake of CECs: The Impact of Functional Group Properties on Plant Uptake Kinetics and Metabolism

1000-1015 Platform 13: A. Simpson, Stanford U.

New Food-Based Disinfection Byproduct of Oleic acid from Chlorine Disinfection during Washing of Spinach and Lettuce

1015-1030 **Questions/Discussion**

1030-1045 *Break*

PFAS and Sources

1045-1100 Platform 14: A. Nickerson, Colorado School of Mines

Simulating impacts of biosparging on release and transformation of PFASs from AFFF-impacted soil

1100-1115 Platform 15: C. Remucal, U. of Wisconsin-Madison

The role of Green Bay tributaries and sediments as a source of PFAS to Lake Michigan

1115-1130	Platform 16: J. Blotevogel, Colorado State U.
	High-Field 21 Tesla FT-ICR MS for PFAS Discovery and Forensic Source Allocation in Impacted Groundwater
1130-1145	*Platform 17: G. Jones, Oregon State U.*
	Opening Pandora's Box: Machine learning applications for chemical forensics and non-target chemical analyses
1145-1200	**Questions/Discussion**
1200-100	*Lunch Break (or Eurofins Live session)*
Biomolecular CECs	
100-145	Keynote: Kim Parker, Washington University in St. Louis
	Environmental Fate of RNA Interference (RNAi) Biopesticides
145-200	Platform 18: H. He, U. of Washington
	Degradation and deactivation of bacterial antibiotic resistance genes during chlorine-based wastewater disinfection:
200-215	**Questions/Discussion**
215-230	*Break*
Ecotoxicology	
230-245	Platform 19: P. Schumann, U. of Wisconsin-Milwaukee
	RNA sequencing reveals potential neurotoxicity biomarkers in Pimephales promelas exposed to wastewater effluent containing a complex pharmaceutical mixture
245-300	Platform 20: S. Stinson, U. California-Davis
	Effects of agricultural surface water and associated contaminants on mortality, gene expression and behavior in aquatic invertebrates and fish
300-315	Platform 21: C. Prasse, Johns Hopkins U.
	Reactivity-directed analysis: A novel approach for the identification of toxic organic chemicals formed during water treatment with chemical oxidants
315-330	**Questions/Discussion**
330-345	*Break*
Wildfire Risks and CEC Treatment	
345-400	Platform 22: E. Hoh, San Diego State University
	Non-targeted Analysis of Stormwater Runoff Following the 2017 Northern San Francisco Bay Area Wildfires
400-415	Platform 23: R. Scholes, U. British Columbia
	Biotransformation of wastewater-derived trace organic contaminants in openwater treatment wetlands for wastewater polishing and reverse osmosis concentrate treatment
415-425	**Questions/Discussion**
425-430	*Break*
Lightning Talks, Posters, Networking, and Community	
430-500	**Lightning Talks (5 Min Each)**
	Kidd et al.
	Municipal wastewater-derived bacteria and changes to the microbiomes of aquatic and riparian invertebrates downstream of outfalls
	Gadhamshetty et al.
	Antibiotic-resistant microbes as emerging contaminants in wastewater infrastrcuture: Initial studies in western South Dakota, USA
	Borch et al.
	Reusing oil and gas produced water for agricultural irrigation
	Shahriar et al.
	Modeling the fate of ionic pharmaceutical and personal care products (iPPCPs) in soil-plant systems: pH and speciation
	Lovin et al.
	Developing a comparative understanding of the aquatic toxicology of (+/-) anatoxin-a and (+) anatoxin-a in two common fish models
	Webster et al.
	Impact of widespread urban burning during the 2018 Camp Fire California, on contaminants of emerging concern in watersheds
500-510	**Concluding Remarks**
	Thanks and Acknowledgments
600-610	**Student Presentation Award Winners Announcements**
	Recogizing excellence in our young scientists!!
510-700+	**Open Discussion, Virtual Poster Session, Asynchronous Talks, and Networking**

Posters and Unscheduled Papers

Posters

Adaeze Ruth

Suitability of Lateritic Soil for Road Construction A Means Carbo Sequestration and Energy Management

Behrens et al.

Towards a Tiered Approach to Assess Effects of Contaminant Mixtures in Urban Streams

Chaplin et al.

Towards Predictive Models for Virus Inactivation by Chlorine

Curtis et al.

Copper phosphate nanosheets as an agrofertilizer: implications for environmental behavior, transformation, risk towards aquatic species

Goodluck Eberechi

Environmental assessment of heavy metals contamination of soil in selected dumpsites in Niger delta, Nigeria.

Gallimore-Repole et al.

Assessing Haloacetonitrile Formation from Model Nitrogenous Precursors

Henke et al.

Age matters? Examining age-specific behavior and proteomic responses of zebrafish (Danio rerio) to a model toxicant

Kamat et al.

Use of UV-LED based halogen advanced oxidation processes for removal micro-pollutants from DOMrich bioreactor effluent

Knutson et al.

Computational approaches for the prediction of environmental transformation products: Chlorination of steroidal enones

Lao et al.

Quantitatively measuring freely dissolved cyanotoxins with diffusive gradients in thin films (DGT) samplers in recreational lakes of Southern California, USA

Mitchell et al.

Evaluating permeable pavements as a stormwater management technology for tire wear particle attenuation

Numan et al.

Engineering application of soluble biochar for pollutant removal

Unscheduled Papers

Ahmed et al.

A liquid chromatography tandem mass spectrometry method for the quantification of selective analgesics and their metabolites in wastewater influent

Bai et al.

PFAS in Nevada water systems: occurrence, treatment, bioaccumulation, and interaction with microplastics

Barber et al.

Watershed-Scale Integrated Ecotoxicological Assessment: Implications of Exposure to Complex Inorganic and Organic Chemical Mixtures

Bothfield et al.

Pharmaceuticals and Contaminants of Emerging Concern in Washington’s Wastewater: Ecology’s Prioritization and Mitigation Strategy

Bradley et al.

Regulated and Emerging Contaminants in Tapwater: Point-of-Use Mixture Exposures and Potential Effects Screening

Brander et al.

Microplastic Pollution in California: Using Scientific Guidance to Inform a Precautionary Framework that Assesses and Addresses Risks to Marine Ecosystems

Chaubey et al.

Modified Biochar for Sorptive Removal of Emerging Contaminant

Chen et al.

Halogen Radicals Contribute to the Halogenation Chemical Additives in Hydraulic Fracturing Fluids

Chin et al.

Physicochemical and Organic Matter Partitioning Properties of Novel Brominated FlameRetardants

Chow et al.
  Evaluating pesticide application data to determine the drivers of aquatic pesticide pollution in the Western Cape, South Africa
Cunningham et al.
  Detrimental effects of tire wear particles and leachate on model organisms Danio rerio and Daphnia magna
Dutch et al.
  Quantification and spatial distribution of pharmaceuticals, personal care products, and perfluoroalkyl substances in Puget Sound sediments from 2010 through 2019.
Elsayed et al.
  Mathematical model development and calibration for microplastic reduction using hydrolytic enzyme
Foster et al.
  Toxicity of Novel Tire-derived Chemical 6PPD-quinone to Coho Salmon (Oncorhynchus kisutch) under Varying Environmental Conditions
Ghorbani Gorji et al.
  Characterisation of the chemical contents of per and polyfluoro substances in aquatic environmental systems using non-target screening and passive sampling technique
Givens et al.
  The First Statewide Assessment of Antibiotic-Resistant Bacteria and Antibiotic-Resistance Genes in Iowa’s Streams
Gray et al.
  Determination of perfluoralkyl substances in waterby direct injection of matrix-modified centrifuge supernatant and LC/MS/MS
Herzog et al.
  Tailoring stream restoration designs to optimize removal of stormwater contaminants
Hu et al.
  Transformation Product Formation Upon Heterogeneous Ozonation of the Tire Rubber Anti-Oxidant N-1,3-Dimethylbutyl-N-Phenyl-P-Phenylenediamine
Hutton et al.
  Influence of salinity on pyrethroid toxicity: behavior in a model estuarine organism (Menidia beryllina)
Jämting et al.
  Comparing the limits of detection of different Fourier transform infrared spectroscopy techniques for the detection, quantification and identification of microplastics
Jones et al.
  Ethylene oxide emissions and risk of breast cancer and Non-Hodgkin lymphoma in a large U.S. cohort
Kotchey et al.
  Potential for Bioelectrochemical Degradation of BPA
LeFevre et al.
  Alteration of the Neonicotinoid Insecticidal Pharmacophore Drives Differences in Parent and Product Sorption: Experimental, Field, and Modeling Results
LeFevre et al.
  Spatial and Temporal Variability of Complex Pharmaceutical Mixtures and their Impacts in a Temperate-region Wastewater Effluent Dominated Stream
Li et al.
  Virus emissions from toilet flushing: comparing urine diverting to mix flush toilets
Lokesh et al.
  Critical role of semiquinone in the reductive dehalogenation
Maizel et al.
  Effects of Wear Processes on Per- and Polyfluoroalkyl Substances in Firefighter Turnout Gear Textiles
McFadden et al.
  Microbial biotransformation of dichloroacetamide herbicide safeners in river sediment microcosms
Meade et al.
  In vitro predictions vs. in vivo reality: Molecular impacts of exposure to WWTP effluent in zebrafish embryos are partially predicted from aggregated ToxCast data
Ohoro et al.
  Occurrence and distribution of pharmaceuticals in surface water and sediment of Buffalo and Sundays River estuaries, South Africa and their ecological risk assessment

Okaikue-Woodi et al.

Synthesis of ferrate-coated sand and application for urban stormwater treatment

Peter et al.

Assessing Reliability of Non-Targeted High-Resolution Mass Spectrometry Fingerprints for Quantitative Source Apportionment in Complex Matrices

Pinkard

Hydrothermal Processing for Emerging Contaminant Treatment

Ray et al.

Catalytic, reductive defluorination of per- and polyfluoroalkyl substances by vanadium carbide MXenes and hydrogen peroxide

Schulze et al.

Combining passive sampling sorbents and Non-Target Analysis (NTA) for comprehensive characterisation of contaminants of concern in environmental water systems

Shi et al.

Quantifying Untargeted Metabolomic Changes in Watersheds and the Contribution of Putative Environmental Drivers

Szczuka et al.

Chloride enhances viral genome reaction rates at conditions relevant to water treatment.

Schlenk et al.

Sediment transfer and toxicity of novel halogenated disinfection byproducts of the pharmaceutical agent, gemfibrozil to marine organisms.

Tillema et al.

Proposed Process for Thermal Destruction of PFOA and PFOS by Municipal Solid Waste Derived Biochar

Un Jan Contreras et al.

The Environmental Fate and Effects of Antibiotic Resistance Genes and Small Interference RNAs From Genetically Modified Crops

Van Brocklin et al.

Investigating Sea Otter Exposure to Microplastics Using Spraint and Diet Analysis

Zhang et al.

RNA hydrolysis at mineral-water interfaces

Zhao et al.

Biotransformation of Current-Use Progestins Dienogest and Drospirenone in Laboratory-Scale Activated Sludge Systems

Zheng et al.

Direct injection analysis of oxypurinol and metformin in wastewater using hydrophilic interaction liquid chromatography coupled to tandem mass spectrometry

Zvekic et al.

Direct Analysis of Trace Contaminant-Microplastic Sorption Phenomena with Membrane Introduction Mass Spectrometry

KEYNOTE ABSTRACTS

Emcon: International Conference on Emerging Contaminants

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Pharmaceuticals and personal care products in the agriculture-food: Current knowledge and future perspective

Evyatar Ben Mordechay, Tomer Malchi and Benny Chefetz

Department of Soil and Water Sciences, Institute of Environmental Sciences, Faculty of Agriculture, Food and Environment, Hebrew University of Jerusalem, Israel

Global water stress, a consequence of population growth, climate change, and increasing demand for food, has increased the reliance of agriculture on water reuse. Water reuse is a growing practice worldwide, e.g., in southern Europe (Cyprus, Greece, Italy, Spain), the United States (California, Colorado, Florida), Mexico, and mainly in countries in the Middle East. The agricultural sector's dependence on water reuse is a mounting global reality with unknown potential environmental and human health consequences.

Wastewater-treatment plants use physical, biological and chemical processes to remove conventional pollutants from sewage. In accordance with government regulations, treated effluents are discharged into the environment or reused for agricultural purposes. The inability of conventional treatment plants to remove various organic contaminants results in their omnipresence at low concentrations in treated effluents. Hence, the use of treated wastewater for irrigation exposes agricultural soil and crops to active pharmaceuticals and personal care products. The presence of pharmaceuticals in crops further introduces these compounds into the food chain and results in involuntary human exposure and subsequent unknown consequences.

This paper examines research progress and challenges, highlighting the potential value of leveraging existing knowledge from research on other chemicals such as pesticides and pharmacology. A process-driven scheme is outlined for future research efforts on pharmaceuticals and personal care products and other analogous emerging contaminants in the agriculture-food system.

Environmental Fate of RNA Interference (RNAi) Biopesticides

Kimberly Parker, Energy, Environmental, and Chemical Engineering
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Abstract

RNA interference (RNAi) is a biological process in which double-stranded RNA (dsRNA) directs the degradation of homologous messenger RNA (mRNA), preventing the synthesis of proteins. In agriculture, several RNAi-based products have been developed using dsRNA as active agents to protect crops from pests (i.e., dsRNA biopesticides). The ongoing development and risk assessment of dsRNA biopesticides necessitates a fundamental understanding of the environmental fate of dsRNA molecules. In this presentation, I will share new methods that our group has developed to investigate dsRNA fate in agricultural soils and surface waters. Then, I will discuss results from our research investigating dsRNA adsorption, biological degradation, and abiotic degradation in these matrices. Throughout the presentation, I will highlight the unique properties of biomacromolecular pollutants like dsRNA biopesticides that alter their detection and fate relative to more traditionally studied low molecular weight chemicals.

Bio

Dr. Kimberly Parker is an assistant professor of Energy, Environmental and Chemical Engineering at Washington University in St. Louis. After earning her PhD at Stanford University, she was then awarded a Marie Curie Individual Fellowship (European Commission) to conduct research at ETH Zurich (Switzerland) prior to joining the faculty at Washington University. Her research has been recognized with honors including the Best Science Paper of the Year published in Environmental Science & Technology (2016), the Paul V. Roberts/AEESP Outstanding Doctoral Dissertation Award (2017), and an NSF CAREER Award (2021).

The Multi-Dimensionality of Microplastics – And How That Influences Their Fate and Effects in Aquatic Ecosystems

Chelsea M. Rochman
Ecology and Evolutionary Biology,
University of Toronto
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Abstract

Today, we are inundated with media about ubiquitous contamination of microplastic in our global ecosystems. Over the last decade, the amount of research and attention regarding the topic has elevated microplastic pollution to the global stage – setting priorities for research and policy. The story of microplastic pollution began in the remote central gyres of the oceans. Now we know that plastic debris is ubiquitous across all oceans, ecosystems, habitats and food webs – including in seafood and sea salt. In addition to understanding contamination, researchers have expanded their breadth of questioning towards the sources, fate, transformations and effects of plastic pollution. A deeper understanding has revealed the many ways in which plastic debris interacts with planetary cycles and affects physical and biological processes. This talk will provide an overview of microplastics and share recent research to better understand the fate and transport of microplastics in food webs (e.g., whether microplastics bioaccumulate and biomagnify) and how microplastics and their associated chemicals impact ecosystems across all levels of biological organization.

Occurrence and Temporal Trends of the Coho Salmon Toxicant 6PPD-Quinone in Urban Creeks

Zhenyu Tian, Melissa Gonzalez, Craig Rideout, Haoqi Zhao, Ximin Hu, Edward P. Kolodziej

Current: Chemistry and Chemical Biology, Northeastern University
Previous: Center for Urban Waters, Tacoma, WA
z.tian@northeastern.edu

Abstract

Coho salmon in the Pacific Northwest exhibit acute mortality after exposure to urban stormwater. Our recent work identified the coho salmon toxicant (6PPD-quinone) as an important transformation product of the ubiquitous tire rubber additive "6PPD". 6PPD-quinone is acutely toxic to juvenile coho salmon and was detected in all examined highway runoff samples and some stormwater-impacted urban creek water samples. Building from our previous semi-quantification methods, we developed and validated a more accurate quantification method using HPLC-MS/MS (triple quadrupole) and isotope-labeled internal standard normalization. To better understand the environmental occurrence and temporal trends of 6PPD-quinone during storm events, we collected stormwater samples from three urban creeks across seven rain events and during baseflow conditions. At one site (Miller Creek) an ISCO sampler was used to automatically collect high-resolution temporal profile samples (one sample per hour). Grab samples were collected from Longfellow Creek and Thornton Creek to confirm the widespread occurrence of the 6PPD-quinone and understand occurrence trends. Hydrographs and pollutographs of 6PPD-quinone were paired to analyze the factors influencing its environmental transport. This work helps us to understand the environmental occurrence and fate of 6PPD-quinone and other roadway runoff contaminants while providing insights for stormwater treatment and salmon conservation efforts.

Short Biography

Zhenyu Tian is an assistant professor at Northeastern University. He worked as a postdoctoral research scientist at the Center for Urban Waters, University of Washington Tacoma, applying non-target screening to identify emerging contaminants in stormwater, marine water, and biota, and to evaluate engineered treatment systems. He received his Ph.D. from University of North Carolina in 2018, studying the transformation products and co-occurring pollutants of PAHs in contaminated soil.

PLATFORM ABSTRACTS

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Plastics contamination in archived biosolids from 1950 to 2016

Elvis D. Okoffo[1]*, Erica Donner[2], Steve P. McGrath[3], Benjamin J. Tscharke[1], Jake W. O'Brien[1], Stacey O'Brien[1], Francisca Ribeiro[1,4], Stephen D. Burrows[1,4], Tania Toapanta[1], Cassandra Rauert[1], Saer Samanipour[5,6], Jochen F. Mueller[1], Kevin V. Thomas[1]

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Presentation type: Oral

*Speaker and corresponding author: e.okoffo@uq.edu.au

Abstract

Plastics are ubiquitous contaminants that leak into the environment from multiple pathways including the use of treated sewage sludge (biosolids). Seven common plastics (polymers) were quantified in the solid fraction of archived biosolids samples from Australia and the United Kingdom from between 1950 and 2016. Six plastics were detected, with increasing concentrations observed over time for each plastic. Biosolids plastic concentrations correlated with plastic production estimates, implying a potential link between plastics production, consumption, and leakage into the environment. Prior to the 1990s, the leakage of plastics into biosolids was limited except for polystyrene. Increased leakage was observed from the 1990s onwards; potentially driven by increased consumption of polyethylene, polyethylene terephthalate and polyvinyl chloride. We show that looking back in time along specific plastic pollution pathways may help unravel the potential sources of plastics leakage into the environment and provide quantitative evidence to support the development of source control interventions or regulations.

Keywords: Plastics; Sewage sludge; Biosolids; WWTPs; Plastic production; Quantification; Pyr-GC/MS

Adsorption of contaminants of emerging concern (CECs) on large and microplastic polyvinyl chloride, polyethylene, and polystyrene

Linda Y. Tseng [1, 2, *], ChanJu You [2], Cecilia Vu [1], Catherine Wang [1], Pitiporn Asvapathanagul [3], and Philip B. Gedalanga [4]

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Abstract

Plastics are synthetic polymers that are light in weight, durable, and resistant to biodegradation. Among several sizes of plastic debris that enter the environment, microplastics are commonly defined as plastics that are less than 5 mm in size. The small size enables the microplastic particles to be ingested by aquatic organisms and raises concerns for aquatic life. However, the potential risks of microplastic accumulation in aquatic organisms are still being investigated by researchers for details on their fate and effects in the ecosystem. In this study, we investigated the adsorption of contaminants of emerging concern (CECs; diclofenac, atenolol, ibuprofen, acetamidophenol, bisphenol A, 2-mercaptobenzothiazole) onto some of the most commonly found plastics in the environment, polyvinyl chloride (PVC), polyethylene (PE), polystyrene (PS). We examined in the lab the isothermal adsorption of these chemicals on large and micro-sized plastics in water for seven days. Large PVC did not adsorb much CECs compared to the micro-PVC and both sizes of PE and PS. In addition, all three plastics, regardless of size, retained some diclofenac and bisphenol A immediately. We attempted modeling a pseudo-first order to find the rate, k, of adsorption for diclofenac and bisphenol A on large PE, and we found their k to be 0.201 and 0.218 d^{-1}, respectively. The results of this study highlight the potential for CECs to be retained on common plastics and, subsequently, the risk for aquatic organisms to be exposed to a higher concentration of CECs when ingesting either the large or micro-sized plastics.

Signal decrease of microplastic polypropylene due to simulated weathering during quantification analysis with Pyrolysis Gas Chromatography Mass Spectrometry

Tania Toapanta[1], Elvis D. Okoffo[1], Stacey O'Brien[1], Stephen Burrows[1,2], Francisca Ribeiro[1,2], Michael Gallen[1], Sarah Ede[3], John Colwell[3], Andrew Whittaker[4], Kevin V. Thomas[1], Sarit Kaserzon[1]

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Interested in presenting an oral presentation

Degraded or weathered microplastics possess characteristic properties different from its virgin counterparts. Comprenhensive assessments on how these properties influence variability when quantitative analysis is performed by Pyrolysis Gas Chromatography/Mass Spectrometry (Pyr-GC/MS) have yet to be performed. This study assessed the accelerated laboratory weathering (0.68 W/m^2) of micro-sized isotactic polypropylene of two different forms; beads (size: ~5 mm; shape: oval) over an exposure time series of up to 80 days and fragments (size: 250-500 µm and 500-1000 µm, shape: irregular) over an exposure time series of up to 37 days). The photo-oxidation of the microplastics was confirmed via Fourier-transform Infrared - Attenuated Total Reflection (FTIR-ATR), scanning electron microscopy (SEM), and differential scanning calorimetry (DSC). We examined whether photo-oxidation affects quantitative measurements using a double shot Pyr-GC/MS method, and identify weathering markers (oxidation products) at a lower pyrolysis temperature.

The degradation rate was faster for fragments compared to beads, possibly due to higher surface area. Comparison of chromatograms between virgin and weathered polypropylene showed no evident qualitative changes in the oligomer mixture, yet there were visible quantitative changes. Specifically the pyrolysis product, 2,4-dimethyl-1-heptene (trimer), showed a signal reduction of 49% for beads and 42% for fragments (after 80 and 37 days, respectively). Six weathering markers were observed to overall increase with higher exposure days. These study suggest that weathering processes are affecting quantitation of isotactic polypropylene microplastics by Pyr-GC/MS and highlights the need for further analytical comparisons between virgin and weathered microplastics in order to avoid underestimation of microplastic exposure studies.

Using Cell Cytometry and Raman Spectroscopy to Characterize Microplastic Particles < 300-Microns in Water Samples.

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The environmental hazards associated with microplastics come from the physical accumulation of particles in a myriad of organisms, as well as the increased exposure of life forms to chemicals and biofilm-associated microorganisms associated with polymer surfaces. Concern is growing over the presence of microplastic particles < 10-micron that are found in water, soils, and air samples. Typically, optical microscopy is used to quantify and chemically characterize larger microplastic particles (≥50 microns), however smaller particle analysis becomes extremely challenging and is fraught with operator bias. To address the need for an accurate, rapid, unbiased, and quantitative characterization of microplastics ≤ 300 microns, multistage fractionation was used to separate particles into less than 300- and 70-micron subsamples, followed by counting using a cell cytometer. This procedure allows for the quantification of microplastic particles as small as 1-micron and allows for replicate measurements to determine the statistical distributions of particle size and mass. Multiple Raman spectral scans of the subsamples, followed by spectral deconvolution, provides chemical information related to polymer composition and degree of oxidative weathering. Known amounts of polyethylene microspheres of a specific diameter are added as an internal standard to samples as they are easily distinguished from microplastic particles and provide a measure of percent recovery. This methodology was used to characterize microplastics ≥ 1-micron in size present in real-world water samples ranging from agricultural runoff with a high suspended clay content to samples collected from open water columns.

The Internalization And Sub-Lethal Effects Of Tire Wear Micro And Nanoparticles On Two Estuarine Indicator Species

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Keywords: Road wear, tyres, behavior, growth, salinity, microplastics, nanoplastics, fish, crustacean

ABSTRACT

Plastic debris is a ubiquitous source of pollution in estuarine ecosystems. Micro (< 5 mm) and nanoplastics (< 1µm) are known to have adverse effects on the habitats, diets, and physiologies of aquatic organisms, but questions remain about the relative risk across salinities, concentrations, and sizes. Less is known about the effects of tire wear particles (TWP), recently defined as plastic debris, as an aquatic contaminant. TWP is generated from automobile traffic, composed of complex mixtures of oil, plastic, steel, and additives and has been detected in coastal and estuarine habitats. Herein, early life stages of estuarine indicator species inland silverside (*Menidia beryllina*) and mysid shrimp (*Americamysis bahia*) (1 day pre-hatch – 4 days post hatch; 7-14 days post hatch, respectively) were exposed to three concentrations of TWP (60, 6000, and 60,000 particles/mL) at micro and nano size fractions with leachate across 5-25 ppt salinity gradient. *M. beryllina* and *A. bahia* had significantly altered swimming behaviors, such as freezing, in zone duration and total distance moved, that could lead to an increased risk of predation and foraging challenges in the wild. Both *A. bahia* and *M. beryllina* growth was reduced in a concentration dependent manner when exposed to micro TWP, whereas *M. beryllina* demonstrated reduced growth only when exposed to nano TWP. Salinity related TWP internalization were also observed with both taxa. *A. bahia* and *M. beryllina* had significantly higher particle ingestion at 15 PSU following micro TWP exposure. The presence of adverse effects in *M. beryllina* (growth at micro TWP and behavior) and *A. bahia* (behavior) *indicate* that even at current environmental levels, which are expected to continue to increase, aquatic ecosystems are likely experiencing negative impacts from TWP pollution.

Occurrences of tire rubber derived contaminants in cold-climate urban runoff

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Abstract

Recent findings that the quinone transformation product of a common tire rubber antioxidant (N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine, 6PPD) is ubiquitous and acutely toxic in stormwater impacted streams has highlighted the need for a better understanding of contaminants related to tire rubber in urban runoff. This study represents the first report of 6PPD-quinone and other tire rubber related compounds in stormwater and snowmelt of a cold-climate Canadian city. Snowmelt and stormwater were sampled across the City of Saskatoon in 2019 and 2020. Of the five target compounds, the common rubber vulcanizing agent N,N'-diphenylguanidine (DPG) was most abundant, with average concentrations of 60 µg L^{-1} in stormwater and 1 µg L^{-1} in snowmelt. Peak concentrations of DPG reached >300 µg L^{-1}, equivalent to loadings of >15 kg from a single rain event. These concentrations of DPG represent some of the highest reported in urban runoff globally. 6PPD-quinone was detected in 57% of stormwater samples with a mean concentration of ≈600 ng L^{-1} (2019) and in >80% of snowmelt samples with mean concentrations of 80 – 370 ng L^{-1} (2019 and 2020). Concentrations of 6PPD-quinone exceeded the acute LC_{50} for coho salmon (0.8 – 1.2 µg L^{-1}) in >20% of all stormwater samples.

EMCON 2021 Abstract – Cassandra Rauert

Abstract Title:

Linking occurrence of tyre road wear particles (TRWP) and tyre additive chemicals in Australian urban water cycles

Authors:

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Presentation Type:

Oral Preferred

Abstract:

Tyre road wear particles (TRWP) have been suggested as one of the primary sources of microplastics to the environment. Further concern arises from chemical additives incorporated into the tyre material that can leach into the surrounding environment. These chemicals have demonstrated links to aquatic toxicity including the vulcaniser hexa(methoxymethyl)melamine (HMMM) and the antioxidant derivative 6PPD-quinone, with particularly high concentrations in stormwater runoff. The current study investigated inputs and co-occurrence of TRWP and a wide range of tyre additive chemicals (including HMMM and 6PPD-quinone) in an Australian urban water cycle during storm events. Grab samples were taken from a creek in Brisbane, AUS, which has direct traffic inputs from two major artery roads. Samples were filtered to remove particles >0.7µm and the residue analysed with Pyrolysis gas chromatography mass spectrometry for markers of TRWP, including synthetic and natural rubber. The filtrate was extracted and analysed with LC-MSMS for a range of tyre related chemicals (n=16), including HMMM and 6PPD-quinone.

A similar chemical profile was seen throughout every storm event, enabling a fingerprint of Brisbane traffic related chemical inputs to be established. The chemicals of high concern, HMMM and 6PPD-quinone were detected in all samples, all be it at concentrations lower than those previously reported to have links with aquatic toxicity. Furthermore, the mass of synthetic rubber (as a proxy for TRWP) in the samples correlated with concentrations of the tyre related chemicals, providing evidence of a direct link between TRWP inputs and chemical tyre additive profile in an urban water cycle.

Quantification of tire and road wear particles and associated road pollutants in a Norwegian tunnel system

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Abstract

Road tunnels have been investigated as road pollution hotspots for several decades and are well-known for their discharge of polluted tunnel-wash water to nearby water recipients. Road tunnels are semi-closed systems which make them ideal for studying known contaminants such as particles (TSS), metals, and new and emerging organic compounds such as rubber, benzothiazoles and antiozonants from tire and road wear. The present study aimed to explore the distribution of contaminants in different tunnel compartments such as road surface before/after wash, gully-pots before wash, tunnel wash water before/after treatment by sedimentation. Styrene Butadiene Rubber, Butadiene Rubber and Styrene Butadiene Styrene (SBR+BR+SBS) from tire and road wear particles were quantified using Pyrolysis Gas Chromatography Mass Spectrometry. A subset of samples was analyzed for metals (zinc, nickel, copper, lead, antimony, wolfram, sulphur), TSS, particle size distribution and organic compounds (including 6-PPD-quinone). For the road surface samples, the results from before and after road cleaning show that insufficient cleaning of the tunnel may cause redistribution of rubbers to other areas. The treatment of tunnel wash water showed a retention of 66% for the rubber and 71% for TSS. A strong linear relationship (R^2-adj=0.88, $p<0.0001$) between rubbers and TSS (Fig. 1) was established. For the metals analyzed, the retention ranged from 38% (lead) to 60% (zinc and copper). We will present an assessment of the relationship between rubbers, tires, road particles, particle-size distribution and pollutants in the presentation and discuss how these can be used to monitor road runoff.

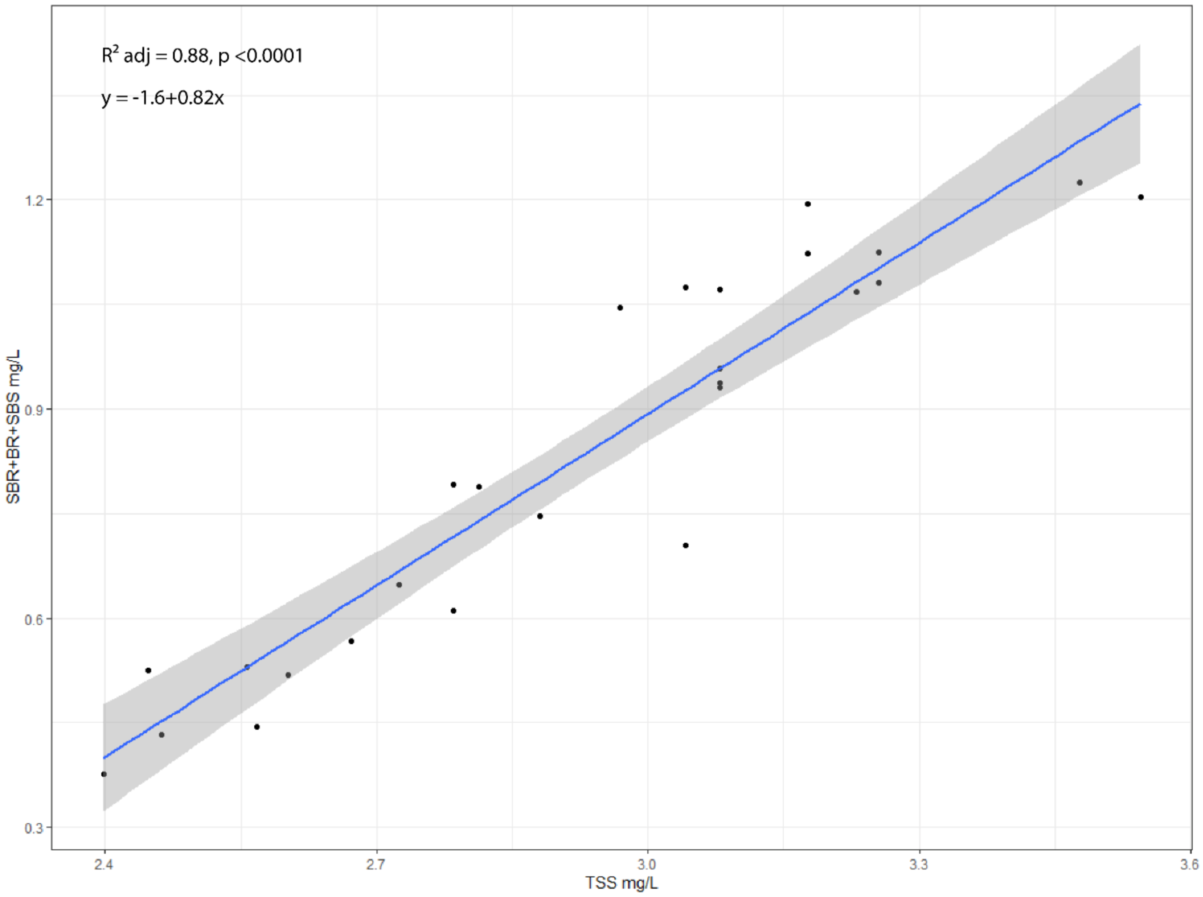

Figure 1. Linear relationship between the rubbers SBR+BR+SBS (mg/L, log10) against total suspended solids (TSS, mg/L, log10). The grey area depicts the 95% confidence interval.

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Title: Model analysis and visualization of 6PPD-quinone fate and transport in Longfellow Creek watershed, Seattle, USA.

Abstract: Transport of materials from the landscape controls nearshore water quality in most estuarine and coastal ecosystems, including Puget Sound. A prevailing assumption is that nearshore and coastal water quality can be improved through effective land use policies that explicitly include minimizing pollutant runoff. Examples include requirements that green infrastructure such as rain gardens, and gray infrastructure such as detention ponds, be included in new and updated development projects. Developing such policies and strategies requires understanding the relationships between the kinds, amounts and spatial distribution of green and gray infrastructure and resulting loadings of water, sediments, pathogens, and chemical pollutants. This presentation focuses on applications of the US EPA's VELMA ecohydrological model for assessing the effectiveness green and gray infrastructure improvements for reducing stormwater contaminant loads to Seattle's Longfellow Creek. This creek, like many other urban creeks draining to Puget Sound, experiences high rates of coho salmon prespawn mortality associated with lethal concentrations of 6PPD-quinone, a breakdown product of 6PPD contained in tire-wear particles (Tian et al. 2020). Details of the hydrological and biogeochemical processes controlling spatial and temporal dynamics of 6PPD-quinone fate and transport from points of deposition to stream and estuary are poorly understood. Here we present initial VELMA model results to elucidate these processes for the Longfellow Creek watershed (1,087 ha). Results include high-resolution (10-m) spatiotemporal animations of 6PPD-quinone fate and transport for various alternative green and gray infrastructure treatments.

Comparison of Organic Chemical Contributions to Receiving Waters from Discharge of Multiple Reuse Waters and Potential Concern to Aquatic Organisms and Human Health

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Given the growing global water shortage, municipalities and water-management agencies worldwide are increasingly using municipal wastewater effluent, urban stormwater, and agricultural runoff as source waters for various water reclamation/reuse purposes. To investigate this topic, reuse water samples of wastewater treatment plant (WWTP) effluent used for irrigation, urban stormwater runoff, and rain-induced agricultural runoff from effluent-irrigated and non-irrigated corn fields were collected during the 2019 growing season and analyzed for a comprehensive suite of 644 organic chemicals. In addition, upstream river water samples were collected during downstream reuse-influenced discharge events to assess relative organic contributions to receiving surface water from discharge of specific reuse water types. Corn plant samples were also collected at harvest to assess contaminant uptake into harvest corn from wastewater reuse practice. Reuse waters contained a complex mixture of organic contaminants including disinfection by products, prescription pharmaceuticals, industrial chemicals, household chemicals, nonprescription pharmaceuticals, polyaromatic hydrocarbons, biogenic hormones, and pesticides. Each reuse water had a unique contaminant profiles that contributed substantial (and varying) loads to receiving surface waters during sampled discharge events. Potential implications for aquatic and human health from WWTP-effluent-irrigation to agricultural fields include contributions of estrone (hormone) and imidacloprid (neonicotinoid insecticide) to receiving surface water and plant uptake of quinolone antibiotics (ciprofloxacin, norfloxacin) and DEET in harvested corn entering the food web.

The first comprehensive chemical and biological characterization of wastewater from food, beverage, and feedstock processing facilities across the U.S.

Process wastewater from food, beverage, and feedstock facilities (FPWW), although regulated, are an under-investigated environmental contaminant source. During phase I (July to November 2018) FPWW from 23 facilities in 17 U.S. states were sampled and demonstrated to contain a plethora of chemical and microbial contaminants. Of 576 analyzed organics, 186 (32%) were detected at least once, with as many as 48 detected in a single FPWW sample. In addition, elevated concentrations commonly observed exceeded 1 $\mu g\ L^{-1}$ with a maximum of 143 $\mu g\ L^{-1}$ (6:2 fluorotelomer sulfonate). Cumulative per/polyfluoroalkyl substances concentrations up to 185 $\mu g\ L^{-1}$ and elevated pesticide transformation product concentrations (e.g. methomyl oxime, 40 $\mu g\ L^{-1}$; clothianidin TMG, 2.02 $\mu g\ L^{-1}$) were observed. Despite 48% of FPWW receiving disinfection prior to discharge, bacteria resistant to third-generation antibiotics were found in each facility category and multiple bacterial groups were detected in all samples, including Total Coliforms. Exposure-activity ratios and toxicity quotients exceed 1.0 in 13 and 22% of samples, respectively, indicating potential biological effects and toxicity associated with the discharge of FPWW. While the results document that FPWW is a substantial source of extensive mixtures of chemical and microbial contaminants discharged to receiving surface waters, the organic contaminant profile differed substantially from that observed in municipal effluent and urban storm water (sources previously documented to also contain extensive mixtures of organic contaminants). During phase II (August to October 2020), a subset of seven of the original facilities were selected to better characterize the environmental exposures and their effects through the sampling of water, bed sediment, and tissue of aquatic organisms (e.g. minnows, crayfish) from the receiving waters both upstream and downstream of the wastewater discharge point. Phase II results will provide a better understanding of potential deleterious effects of chemical and biological contamination from FPWW on the environmental health of receiving waters. Abstract does not necessarily reflect U.S. Environmental Protection Agency views or policy.

Laura E. Hubbard[a], Dana W. Kolpin[b], Carrie E. Givens[c], Brett R. Blackwell[d], Paul M. Bradley[e], James L. Gray[f], Rachael F. Lane[g], Jason R. Masoner[h], R. Blaine McCleskey[i], Kristin M. Romanok[j], Mark W. Sandstrom[f], Kelly L. Smalling[j], Daniel L. Villeneuve[d]

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Probing Putative Transporter-Mediated Plant Uptake of CECs: The Impact of Functional Group Properties on Plant Uptake Kinetics and Metabolism

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ORAL PRESENTATION PREFERRED

Plant uptake and metabolism of contaminants of emerging concern (CECs) can represent critical environmental fate processes or exposure routes. Transporter-mediated active plant uptake is a vastly understudied process compared to passive uptake and applicable to some important CECs. In this work, we studied environmentally relevant model compounds (isothiazolinone biocides, found stormwater from building façades) and benzimidazole fungicides (found ubiquitously from point / NPSs). These compound sets were chosen due to the wide variety commercially available that feature the same base molecule with slight structural changes in functional groups. We documented rapid (within 24 hours for complete or near-complete removal) hydroponic plant uptake by the model plant *Arabidopsis* of four isothiazolinone biocides and multiple benzimidazole fungicides, and observed active uptake rates following Michalis-Menten kinetics with substrate inhibition that was constituently active rather than inducible. A suite of known plant uptake inhibitors did not affect observed kinetics. Functional group differences in isothiazolinone structure (chloro, methyl, aromatic ring) did not significantly impact uptake. In contrast, benzimidazole functional group electrostatic character and position significantly impacted plant uptake rates. Specifically, greatest plant uptake rates occurred with an electron-withdrawing functional group at the 2-position. Electron-donating groups at the 2-position still yielded some plant uptake, indicating possible steric effects between the chemical and transporter protein. An electron-donating group at the 1-position significantly slowed uptake for both benzimidazole and benzotriazole base molecules. We used HRMS-based plant metabolomics to discover novel transformation products and measured upregulated endogenous plant compounds. Pathways included hydroxylation, glutathione conjugation, cyano hydrolysis, and amino-acid conjugation.

New Food-Based Disinfection Byproduct of Oleic acid from Chlorine Disinfection during Washing of Spinach and Lettuce

Authors: Adam M.-A. Simpson; Minjeong Suh; Stephanie Lau; Michael J. Plewa; William A. Mitch

Institution: Stanford University, School of Engineering - Civil & Environmental Engineering Department

Abstract: To prevent cross contamination by foodborne pathogens, processing facilities must disinfect fruits and vegetables with up to 200 mg/L as Cl_2 of chlorine. Chlorine must be hyper-dosed in food washing facilities because chlorine tends to immediately react.
However, following the Food Safety Modernization act of 2011, chlorine exposures must be optimized to prevent the formation of unwanted internal disinfection byproducts (DBPs) isolated inside of washed foods. We have quantified chlorinated food-based disinfection byproducts (F-DBPs) of oleic acid, a fatty acid constituent inside of fruits and vegetables. When spinach and lettuce were exposed to chlorine doses up to 200 mg/L as Cl_2 of chlorine, significant yields of oleic acid chlorohydrins, were measured inside of samples for exposures as short as 2 min at 7.5 ˚C. 9,10-Chlorohydrins increase in yield when spinach was shredded and when chlorine contact time was increased. The cytotoxicity of 9,10-chlorohydrins to Chinese hamster ovary cells was higher than any regulated trihalomethane or haloacetic acid of concern in drinking water. Lastly the additive cytotoxicity of 3-chlorotyrosine, 3,5-dichlorotyrosine and 9,10-chlorohydrins isolated from a survey of vegetables was compared to a daily intake of 2 L of water containing the regulated DBPs chloroform and trichloroacetic acid. The results show that the equivalent mass of vegetables with the same cytotoxicity is lesser than the daily recommended serving of vegetables.

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Simulating impacts of biosparging on release and transformation of PFASs from AFFF-impacted soil

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*prefer oral presentation

Poly- and perfluorinated alkyl substances (PFAS) are frequently present at sites contaminated with fuel-derived components due to the use of aqueous film-forming foam (AFFF). In many cases, remediation for these co-contaminants is implemented prior to knowledge of PFAS contamination. Biosparging is a common remediation technology that injects oxygen into the saturated zone to encourage biodegradation of contaminants such as BTEX. Biosparging alters aquifer redox conditions which may facilitate microbial transformation of polyfluorinated PFAS as an unintended byproduct. It was hypothesized that passing oxygen-saturated artificial groundwater through columns containing PFAS-contaminated soil would alter the release and composition of PFAS. Artificial groundwater sparged with nitrogen or oxygen gas was pumped through four soil columns alongside toluene for 130-280 pore volumes. Column effluents and soils were analyzed for an extensive list of PFASs by high-resolution mass spectrometry. Shortly after the start of sparging, eluted concentrations of several PFASs were greater in the oxygen-sparged columns than in the nitrogen-sparged columns. Mass balance calculations suggested transformation of sulfonamide-based precursors to perfluorinated sulfonamides (i.e. perfluorohexanesulfonamide) in both oxygen- and nitrogen-sparged columns: recoveries of perfluorinated sulfonamides were 158-235% for C3-C6 homologs, while recoveries of several sulfonamide-based zwitterions were low pointing to transformation. These results suggest there are many biologically mediated polyfluorinated transformations under both oxygen- and nitrogen-sparged conditions. Higher concentrations of PFASs eluting from oxygen-sparged columns suggest biosparging has a rapid effect on release of PFASs in saturated soils, which may have important implications for site characterization and remediation.

The role of Green Bay tributaries and sediments as a source of PFAS to Lake Michigan

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Abstract submission for oral presentation:

Identifying and quantifying sources of per- and polyfluoroalkyl substances (PFAS) to the Laurentian Great Lakes is of great importance as this large freshwater system provides drinking water to over 40 million people. However, the importance of PFAS loading to the Great Lakes via tributaries is poorly characterized and the role of sediment as a source or sink of PFAS in these tributaries is largely unknown. We quantified 10 PFAS compounds in water and sediment of 41 tributaries to Green Bay of Lake Michigan, including all major tributaries. Aqueous concentrations (sum of 10 PFAS) range from 4 – 1,310 ng/L, with the highest concentration and highest percentage of perfluorooctanoate in a small stream impacted by a fluorotelomer aqueous film-forming foam manufacturer near Marinette, WI. Sediment PFAS is dominated by perfluorooctanesulfonate (PFOS), with summed concentrations ranging from 0 – 3,255 ng/kg, and is highest in tributaries that are impacted by industrial activity and airports. Three large rivers (i.e., Fox, Menominee, and Peshtigo Rivers) contribute over two-thirds of the total tributary PFAS loading during the study despite having lower PFAS concentrations than most small streams. Field-derived sediment-water partition coefficients are approximately an order of magnitude higher than laboratory coefficients, but follow expected trends based on PFAS chain length and head group. Desorption experiments show that PFOS rapidly desorbs from riverbed sediments when equilibrated with Lake Michigan water, indicating that sediments may act as a PFAS source if water concentrations are reduced by pollution mitigation methods.

High-Field 21 Tesla FT-ICR MS for PFAS Discovery and Forensic Source Allocation in Impacted Groundwater

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Abstract

Per- and polyfluoroalkyl substances (PFAS) have been widely used in industrial and consumer products due to their heat, oil, and water resistance. PFAS leaching from fire training areas, landfills, wastewater treatment plants and other sources may lead to co-located plume development in impacted groundwater. Here, we demonstrate the unprecedented capabilities of ultrahigh-resolution Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) to characterize complex PFAS contaminations at the molecular level. Groundwater samples were taken at three contaminated sites and analyzed on the world's highest-resolving mass spectrometer. We discovered 300 new PFAS species and 75 novel PFAS classes that were unambiguously identified at <0.2 ppm mass error and based on being members of CF_2 Kendrick mass defect series. Thousands of additional PFAS were detected at varying confidence levels. Unique fingerprinting approaches revealed compositional differences between samples, discriminating between different sources based on compositional variability. This first-of-its-kind application of FT-ICR MS analysis of PFAS and the workflow developed here are critical first steps in cataloguing PFAS associated with different sources as well as in identifying unique marker compounds for fingerprinting that can be targeted in the future on more widely accessible low-resolution mass spectrometers.

Abstract Title:
Opening Pandora's Box: Machine learning applications for chemical forensics and non-target chemical analyses

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Abstract:

Water bodies are chemical data loggers that contain tens of thousands of molecules that are derived throughout a watershed. These molecules represent the sum of all the biological, chemical, and physical processes within a watershed, and we hypothesize that unique chemical signatures, or fingerprints, present within a water sample can be informative of upstream processes. My aim was to extract non-polar organic compounds from water samples at/near chemical sources, and then use high-resolution mass spectrometry (HRMS) data in conjunction with machine learning tools to identify the chemical signatures that are diagnostic of each source. If these diagnostic signatures, or fingerprints, are detected in environmental samples, we can confirm the presence of source-specific discharge in receiving bodies of water. This is particularly advantageous for pollution source tracking where some compounds (e.g., nitrate) are generated from multiple sources. Grab samples were collected and analyzed in triplicate from different sources including headwater streams, agricultural field runoff, animal manure, municipal wastewater, and urban/suburban road runoff. Data from artificial intelligence models indicate that each source is readily distinguishable based on its chemical composition and that 10, 25, 50, and 100 non-target chemical compounds could be isolated as diagnostic chemical fingerprints. Also, these diagnostic chemical fingerprints were detected in high probability in mixed water samples (e.g., creeks). This workflow will be open source and freely available to help managers identify pollutant sources present in receiving water bodies, which will help direct limited resources to projects that maximize water quality improvements.

Degradation and deactivation of bacterial antibiotic resistance genes during chlorine-based wastewater disinfection: Significance of chlorine speciation and application of nucleotide-based kinetic modeling approaches

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Chlorine has been widely applied in wastewater disinfection. While chlorination provides effective inactivation of many microorganisms, including antibiotic resistant bacteria (ARB), less is known regarding its efficacy in degrading and eliminating the biological activities of potentially transmissible nucleic acid sequences associated with ARB and other microorganisms, in particular antibiotic resistance genes (ARGs). In this work, a suite of 23 DNA segments, including from the ARGs *blt*, *mecA*, *van*A, *tet*(A), *amp*C, *bla*$_{\mathrm{NDM}}$, and *bla*$_{\mathrm{KPC}}$, as well as from the 16S rRNA genes of corresponding ARB strains, were employed as disinfection targets to investigate gene degradation kinetics during chlorination of bench- and full-scale wastewater – with chlorine residuals present as either *free available chlorine* (FAC) in low-ammonia wastewater or as *combined chlorine* (primarily monochloramine, NH_2Cl) in high-ammonia wastewater. Rate constants for reactions of FAC and NH_2Cl with target DNA segments were first measured in buffer, then used to calibrate a previously-developed approach for predicting rate constants based solely on gene segment nucleotide contents. Rate constants predicted by this approach were then used to model each gene's degradation during bench-scale treatment in buffer and wastewater matrixes. Kinetics of extracellular and intracellular gene degradation by FAC were well predicted up to ~1–2-$\log_{10}$ elimination, whereas NH_2Cl yielded minimal degradation under all conditions (also agreeing with predictions). ARG degradation during full-scale chlorination at a regional wastewater treatment plant was consistent with bench-scale measurements and predictions, and highlights that chlorination of high-ammonia wastewater (dominated by NH_2Cl) can generally be expected to yield minimal ARG degradation.

Abstract Title:

RNA sequencing reveals potential neurotoxicity biomarkers in *Pimephales promelas* exposed to wastewater effluent containing a complex pharmaceutical mixture

Authors:

Peter G. Schumann, Emma B. Meade, Hui Zhi, Gregory H. LeFevre, Dana W. Kolpin, Shannon M. Meppelink, Luke R. Iwanowicz, Rachael F. Lane, Angela Schmoldt, Olaf Mueller, Rebecca D. Klaper

Abstract:

Current wastewater treatment plant (WWTP) technologies have a variable rate of removal of contaminants of emerging concern (CECs). As a result, discharged effluent results in complex mixtures of these contaminants in receiving streams that vary temporally. Among the most frequently detected CECs in WWTP effluent are pharmaceuticals. As wastewater effluent-dominated streams are becoming increasingly common worldwide, this leads to pseudo-persistent exposure conditions that can negatively impact the aquatic and terrestrial organisms that live in and near these streams. Currently there is a paucity of knowledge on the neurological impacts due to exposure to complex CEC mixtures at environmentally relevant concentrations in real-world scenarios. These knowledge gaps leave incomplete assessments of the hazards and risks from exposure to such CEC mixtures as even sublethal neurotoxicity can lead to alterations in ecologically important behaviors in wildlife. To help better understand the potential real-world neurological impacts of CEC mixture exposure, we performed a 96 h *in situ* exposure of fathead minnows (*Pimephales promelas*) in a temperate-region effluent-dominated stream (i.e., Muddy Creek) near Coralville, Iowa, USA. Caged minnows were placed both 100 m upstream and 100 m downstream of a WWTP effluent outfall. After the 96-h exposure, we performed a total RNA sequencing analysis of the collected brain tissues to assess differential gene expression in male and female fish, separately. This revealed genes that were uniquely expressed in females and in males that were significantly differentially expressed at the downstream site when compared against the upstream site. A portion of such genes overlapped in their expression amongst females and males. Functional enrichment analysis was performed on the differentially expressed genes to better understand their specific biological impacts. These brain-specific transcriptomic effects of WWTP effluent exposure in fathead minnows provides potential novel biomarkers to expand monitoring of environmental effects.

Title: Effects of agricultural surface water and associated contaminants on mortality, gene expression and behavior in aquatic invertebrates and fish

Co-authors/affiliations: Stinson S.A. University of California Davis; Egan, N.E. University of California Davis; Deng X. CA Department of Pesticide Regulation; Hasenbein, S. University of California Davis; Lawler S.P. University of California Davis; Holland, E. CA State University Long Beach; Connon R.E. University of California Davis.

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Abstract Text:

Runoff entering waterways from agricultural and urban areas can introduce influxes of highly toxic, complex chemical mixtures into nearby aquatic habitats, causing rapid changes in water quality. These dynamic mixtures often include emerging chemicals of concern. Our goal was to assess mortality, molecular and behavioral responses of aquatic species to exposure to agricultural runoff. We collected surface water from three sites located in an intensely farmed agricultural region in the Central Coast of California, USA. We conducted acute (96h) exposures to geometric dilutions of water samples using a model fish (*Pimephales promelas*) and a sensitive invertebrate (*Daphnia magna*) species, then measured mortality, gene expression and swimming behavior. Analytical chemistry detected low concentrations of eighteen individual chemicals of concern including several pyrethroids, and emerging chemicals of concern: imidacloprid and chlorantraniliprole. For the two sites with the highest detection levels of chemicals of concern, we found >80% invertebrate mortality (even at low dilutions) and differential expression of genes involved in first line detoxification and general stress pathways (CYP1a), muscular and neuronal function (RYR2, SERCA1) for fish. The behavior of both fish and invertebrates was significantly hyperactive in the same sites, relative to controls. Fish also demonstrated altered photomotor response to light stimuli in the same sites. Behavior is an ecologically important endpoint that may have implications for survival if it affects predator avoidance and/or foraging. These findings suggest that the use of multiple endpoints and testing strategies will greatly improve our ability to predict biological responses in a complex environment.

EmCon 2021

Reactivity-directed analysis: A novel approach for the identification of toxic organic chemicals formed during water treatment with chemical oxidants

Author
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Abstract

Treatment technologies that utilize chemical oxidants such as hydroxyl radicals, ozone and chlorine are now widespread in a variety of water treatment applications, including wastewater, water reuse and drinking water. While these technologies are highly effective in removing organic and microbial contaminants, there is increasing evidence that their degradation can lead to the formation of a large variety of transformation products. The same is true for the reaction of chemical oxidants with dissolved organic matter (DOM), which is typically present in concentrations that are several orders of magnitude higher than those of anthropogenic chemicals. However, assessing the potential health risks that arise from the exposure to these complex chemical mixtures remains very challenging. One of the main reasons is the unavailability of approaches that enable the assessment of the overall toxicity of these mixtures while also providing information about the identity of the responsible toxicants. To address this issue, we developed a novel analytical approach, called reactivity-directed analysis (RDA) which focuses on the detection and identification of organic electrophiles, the largest class of known toxicants. RDA utilizes the molecular toxicity mechanism of organic electrophiles, their reactivity with nucleophilic biomolecules such as proteins, to identify this class of contaminants in oxidative water treatment systems. This talk will discuss the results of laboratory experiments with individual organic contaminants and outline how RDA can be used as a novel tool for the identification of reactive organic electrophiles in complex environmental mixtures.

Non-targeted Analysis of Stormwater Runoff Following the 2017 Northern San Francisco Bay Area Wildfires

Presenter: Eunha Hoh[1]

Co-authors: Daniel Chang[2], William H. Richardot[2], Ezra L. Miller[3], Nathan G. Dodder[1,2], Margaret D. Sedlak[3], Rebecca Sutton[3]

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Oral Presentation

ABSTRACT

The full scope of the ecological damage of wildfires is often hard to assess, in part due to limited information on the types of chemicals introduced to affected landscapes and waterways. The objective of this study was to establish a sampling, analytical, and interpretive framework to effectively identify and monitor contaminants of emerging concern in environmental water samples impacted by wildfire runoff. A non-targeted analysis based on comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC/TOF-MS) was conducted on stormwater samples from watersheds in the City of Santa Rosa and Sonoma and Napa Counties after the three destructive fires during the October 2017 Northern California firestorm. Chemicals potentially related to wildfires were selected from the thousands of chromatographic features detected through a screening method that compared samples from fire-impacted sites versus unburned reference sites. This screening tentatively identified 77 potentially fire-related compounds, and among them, 46 were confirmed by matching mass spectra and GC×GC retention times out of 49 commercially available standards. Of these 46 compounds, 37 had known commercial and industrial uses as intermediates or ingredients in plastics, personal care products, pesticides, and as food additives. Nine compounds had no known uses or sources and may be oxidation products resulting from burning of natural or anthropogenic materials. Preliminary examination of potential toxicity associated with the 46 compounds, conducted via online databases and literature review, indicated limited data availability. Regional comparison suggested that more structural damage may yield a greater number of unique, potentially wildfire-related compounds.

Abstract Title: Biotransformation of wastewater-derived trace organic contaminants in open-water treatment wetlands for wastewater polishing and reverse osmosis concentrate treatment

Authors: Rachel Scholes,[1,4] Michael Vega,[3,4] Jonathan Sharp,[3,4] David Sedlak[2,4]

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Abstract:

Nature-based treatment systems are of increasing interest as communities seek to remove contaminants from stormwater, municipal wastewater effluent, and reverse osmosis concentrate. However, designing nature-based treatment systems for reliable trace organic contaminant removal remains a challenge. This research investigated biotransformation in open-water wetlands, which were developed to remove nitrate and trace organic contaminants from municipal wastewater effluent. A pilot-scale open-water wetland treating reverse osmosis concentrate from a water reuse facility was operated for over two years. Monitoring results indicated the growth of a biomat capable of denitrification and biotransformation of trace organic contaminants. Within one year of startup, removal rates of pharmaceuticals susceptible to biotransformation (i.e., atenolol, metoprolol) were similar to rates observed in open-water wetlands treating municipal wastewater effluent. However, compounds that underwent slower removal in previous open-water wetlands were removed only after approximately twenty months of biomat growth (emtricitabine, trimethoprim) or not at all (sulfamethoxazole) in the wetland treating reverse osmosis concentrate. In addition, estimates of carbon fixation rates indicated that denitrification was limited by the availability of organic carbon in the pilot-scale wetland. Microcosm experiments with wetland biomat indicated that denitrification and biotransformation of trace organic contaminants could be enhanced by introducing carbon amendments. In microcosms amended with wood chips, post-adsorption removal rates of sulfamethoxazole and acyclovir were higher than rates observed in experiments containing only biomat. Microcosms amended with acetate exhibited enhanced removal of nitrate but not trace organic contaminants. These results indicate the potential role of carbon availability in trace contaminant biotransformation and suggest that biotransformation could be enhanced in nature-based treatment systems using low-cost carbon amendments.

Reusing Oil and Gas Produced Water for Agricultural Irrigation

Thomas Borch[1], Hannah Miller[1], Pankaj Trivedi[1], Erin Sedlacko[2], Christopher Higgins[2], Molly McLaughlin[1], Linsey Shariq[3], and Jens Blotevogel[1]

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Produced water (PW) is typically injected into deep disposal wells, however, concerns related to groundwater pollution, water scarcity and sustainability have motivated the industry to develop alternative reuse options. Recently, crop irrigation has emerged as an attractive PW reuse option, but the impact on plant immune response is not known. I will present data from a 3-month greenhouse pot study in which spring wheat was irrigated with different levels of produced water. The wheat leaves were inoculated with either bacterial or fungal pathogens and changes in pathogenesis-related PR-1 and PR-5 gene expression were measured from the leaf tissue. This study provides the first evidence that plant disease resistance is reduced due to irrigation with reused PW, which could have negative implications for food security. Select results from studies related to PW impacts on soil health, and contaminant uptake in wheat will also be presented.

LIGHTNING TALK ABSTRACTS

Emcon: International Conference on Emerging Contaminants

September 13–14, 2021

Virtual Event Hosted by University of Washington

Abstract Title:

Using Spatial and Temporal Patterns in an Urban Sewershed for Prioritization of Nontarget Features

Authors:

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Trace organic constituents (TOCs) such as pesticides and pharmaceuticals have been identified in wastewater entering treatment facilities, creating concern due to their poor removal by conventional wastewater treatment and toxicity potential in receiving environmental waters. However, there is little information regarding sources and temporal trends for these TOCs on a sub-sewershed scale. This study examines 24-h time-weighted composite samples collected monthly from February through December of 2016, at the wastewater treatment plant influent, effluent, ten sub-sewershed laterals, and three locations expected to have high pesticide loads (i.e. pet groomer, pest control operator, and laundromat). All samples were analyzed using both liquid and gas chromatography time-of-flight mass spectrometry (LC-QTOF-MS and GC-QTOF-MS) to comprehensively screen for roughly 3500 suspect chemicals. LC-QTOF-MS data were acquired using electrospray ionization (ESI) in positive and negative modes with All-Ions fragmentation, and two accurate mass MS/MS libraries containing >2000 chemicals were screened. The extracts were run on GC-QTOF-MS in electron impact (EI) mode using a retention time locked method and the spectra were screened against a pesticide library containing exact mass fragments and retention times. Additionally, the samples were aligned in an open source nontarget alignment software, MSDIAL, to create a set of nontarget features. Through careful filtering parameters, abundance normalization, and application of multivariate statistical methods such as principal components analysis (PCA) and hierarchical clustering, we plan to investigate patterns in space, time, and groups of features, as well as prioritize features for further identification efforts.

Antibiotic-resistant microbes as emerging contaminants in wastewater infrastructure: Initial studies in Western South Dakota, USA

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Abstract:

The extensive usage and exploitation of antibiotics among animal and human medications had resulted in a pool of antibiotic resistance bacteria (ARB) that continued to be released to the wastewater systems. As a result, the antibiotic/metal resistant genes evolved as emerging contaminants in the wastewater treatment infrastructures of Rapid City, Western South Dakota. Here, we have provided comprehensive data on the 42 different antibiotic/metal resistance genes detected from the Primary Clarifier of Rapid City Wastewater Treatment Plant. Results showed that 29 antibiotics resistant (ARGs), 6 heavy metal-resistant genes (HMRGs) and 7 integrase genes were detected using microfluidic qPCR. Among them, ARGs include 6 beta-lactamase genes, 7 aminoglycoside/quinolone/macrolide genes and 16 other (erythromycin, tetracycline, vancomycin, streptomycin and rifampicin) ARGs. Besides, HMRGs were resistant towards cadmium, copper, nickel, cobalt, chromium and mercury resistances. In addition, microbial community analysis by illumina sequencing revealed that *Arcobacter* sp, *Acinetobacter* sp. and *Acidovorax* sp. were found to be predominant bacteria from the wastewater samples. These three bacteria are widely reported for multidrug resistance (MDR) and thus their mitigation is crucial. On another note, our research group at South Dakota Mines is involved in mitigating these ARBs and ARGs using a photocatalytic reactive membrane functionalized with a nanofiber mat composed of polyvinylidene fluoride (PVDF) as fiber material, carbon nitride and silver (Ag) nanoparticles. Besides, our group is bridging the knowledge gaps in biofilm engineering and ARG mechanisms using axenic cultures involved in sulfate reduction.

Estimation of microplastics in drinking water: A case study of indirect potable reuse

Swadhina Priyadarshini Lenka[1], *Tahereh Jasemizad*[1], *Iraj Rezapour Balaneji*[1], *Brandon Huang*[1], *Benjamin Campbell*[1], *Colin Whittaker*[1], *Lokesh P. Padhye*[1]*

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Our study used literature-informed modelling to predict the fate of microplastics (MPs) in natural and engineered water systems in the North Island of New Zealand for estimating their contribution in a glass of drinking water of Auckland. The study's focus was on the indirect potable reuse practised in Auckland for water drawn from the Waikato River. Worst-case and best-case scenarios were developed for all estimates. For simplifying calculations involving nonpoint sources of the MPs, assumptions were made to estimate their equivalent contribution as point sources through wastewater treatment plants (WWTPs). Wastewater influent concentrations of MPs were calculated based on the catchment population and treatment volumes. The effluent concentrations were based on the estimated treatment efficiencies at each stage of wastewater treatment. For simulating the fate of MPs along the river length, the riverine transport model was used. MPs were divided across different size ranges with a minimum and maximum particle size of 1 and 100 µm, respectively. 10–50 µm MPs would be most easily transported in the river, while particles <10 µm were assumed to settle after forming hetero-aggregates, and particles >50 µm were assumed to settle directly. By estimating removal of MPs at different stages of the drinking water treatment plant, MPs' concentrations in treated drinking water of Auckland was estimated to be below 30 ng/L, even in the worst-case scenario. Our findings suggested that the amount of MPs consumed through a glass of drinking water in Auckland is negligible. The proposed model could be used for estimating MPs' concentrations in source or drinking waters globally, notably where the occurrence data is lacking.

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Title: Developing a comparative understanding of the aquatic toxicology of (±) anatoxin-a and (+) anatoxin-a in two common fish models

Harmful algal bloom toxins present risks to public health and the environment. Anatoxin-a is a globally found neurotoxic cyanobacterial toxin that affects growth, reproduction, and survival of aquatic organisms. Few studies have examined influences of anatoxin-a on gene expression and behavior with common fish models. Therefore, after performing probabilistic hazard assessments, here we studied larval fathead minnow and zebrafish responses following exposure to (±) anatoxin-a at environmentally relevant, analytically verified concentrations We found duration and distance of fathead minnows swimming at the highest speed (>20 mm/s) was significantly lowered (ANOVA, $\alpha = 0.1$) by (±) anatoxin-a in 0.1, 1, and 1.5 mg/L treatments, while the opposite occurred with zebrafish, which showed increased distance, duration, and changes in movement at the highest speed, though not significant. We examined gene expression focusing on genes related to neurotoxicity, oxidative stress, and DNA damage. While there was little change in zebrafish, fathead minnows showed upregulation in many neurotoxicity related genes, though only *elavl3* was significant (ANOVA, $\alpha = 0.05$) as well as downregulation of *gst* and *cyp3a126*. This suggests fathead minnows may be more sensitive to this toxin based on these endpoints. We subsequently have repeated these studies with (+) anatoxin-a, previously reported as the only enantiomer produced by cyanobacteria and observed differential sensitivities among endpoints and between organisms with high mortality in fathead minnows >0.5 mg/L concentrations and showing a largely refractory response in zebrafish. Comparative understanding of cyanotoxins is necessary to support robust assessments and management of algal blooms.

Municipal wastewater-derived bacteria and changes to the microbiomes of aquatic and riparian invertebrates downstream of outfalls.

Elise Millar,[a] Michael Surette,[b,c] and Karen Kidd[a,d*]

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Microbial communities on or within a host, better known as microbiomes, affect an organism's health due to their roles in nutrient accessibility, immune system function, etc. and shifts in these communities are increasingly linked to diseases. These communities of microorganisms can be affected by a host's diet, environmental conditions and chemical exposures, including pharmaceuticals. Effluents from wastewater treatment plants (WWTPs) contain antibiotics and other contaminants that could negatively impact the microbiome of downstream biota. To assess this, we collected five families of aquatic macroinvertebrates and a riparian predator with high reliance on emergent aquatic insects (Tetragnathidae spiders) from sites upstream and downstream of two WWTPs along the Grand River in southern Ontario, Canada. The microbiomes of whole invertebrates and spiders were analysed following the extraction, nested PCR amplification, and sequencing of bacterial genomic DNA using the V3-V4 hypervariable region of the 16S rRNA gene. Changes in the relative abundance of major phyla, decreases in alpha diversity, and changes in beta diversity were observed among sites in most invertebrate microbiomes. Effluent-derived bacteria were found in the microbiomes of downstream aquatic insects and spiders, but not those collected upstream of these discharges. These bacteria are used in wastewater treatment processes, found in the digestive tracts of humans and other mammals, or are opportunistic pathogens. Overall, these results demonstrated the transport of WWTP-derived bacteria through aquatic ecosystems to riparian predators. Additionally, the microbiome of invertebrates differed from upstream to downstream of WWTPs, which has implications for host health.

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Platform preferred

Condensed Phase Membrane Introduction Mass Spectrometry (CP-MIMS) for direct, time-resolved analysis of 6-PPD and 6-PPD quinone

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Preferred format: Oral presentation

A recently identified ozonation product of a common tire preservative, N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine quinone (6-PPDQ), threatens Coho salmon populations at ng/L concentrations particularly in urban streams in the Pacific Northwest. Sensitive and selective analytical techniques are needed to study the environmental fate and distribution of 6-PPDQ including the identification of multiple sources and potential mitigation strategies. Probing fundamental analytical and environmental questions about 6-PPDQ, such as sample holding time and rate and extent of partitioning to various environmental media are expensive and time consuming to assess using conventional analytical approaches such as liquid chromatography mass spectrometry (LC/MS). Condensed phase-membrane introduction mass spectrometry (CP-MIMS) provides an online separation of hydrophobic analytes from ionic and particulate components in complex samples using a semi-permeable polydimethylsiloxane (PDMS) membrane. A flowing solvent acceptor phase dissolves permeating analytes and is directly infused into a mass spectrometer. Using a direct immersion probe, solution phase concentrations can be monitored in real-time to follow dynamic processes (*e.g.* sorption/desorption). We report the use of CP-MIMS to directly monitor the rate and extent of desorption of 6-PPD and 6-PPDQ at trace (ng/L) concentration from tire dusts generated from new and aged tires. Additionally, sorption of both compounds to several natural sediments with a range of organic carbon content is monitored. The stability of 6-PPDQ samples over a 2-week period with various treatments (filtration, acidification, preservative) will also be discussed. Overall, CP-MIMS represents a powerful complement to conventional analytical strategies particularly for high throughput screening and process monitoring.

Passive Sampling Behavior of Electrospun Nanofiber Mats with Embedded Carbon Nanotubes for Emerging Contaminants in Water and Air

Matthew Nagorzanski, Andres Martinez, Jiajie Qian, and David Cwiertny

We fabricated polymer electrospun nanofiber mats (or ENMs) and tested their ability to function as fast equilibrating passive sampling devices for various emerging contaminants in water and air. The ENMs fabricated are made of polyacrylonitrile and contain embedded carbon nanotubes. Previous work with these materials has shown their ability to sorb various emerging contaminants, e.g. atrazine, and their ability to reach equilibrium in water in less than one day. Preliminary deployments of these ENMs in local Iowa surface water has also resulted in good agreement of atrazine concentration compared to grab samples taken near simultaneously. Nevertheless, questions still remain about how ENMs actually behave in environments with dynamic concentrations of emerging contaminants as would be expected from releases of pollutants into air and water from discharge events. Current work is quantifying the timescales and extent of reversibility of contaminant sorption to ENMs, as well as the ENM response to changes in pollutant concentration over time. Thus far, we have shown that ENM sorption of emerging contaminants is largely reversible, occurring over similar time scales to contaminant uptake. This suggests that results derived from deployed ENMs likely only reflect surface water contaminant concentrations at or within a close time interval during deployment. Current work is also focused on use of these materials for monitoring pesticide drift with an initial focus on their equilibrium uptake of pesticides atrazine and dicamba from air. Together, this work is helping inform how ENM samplers can represent a feasible passive sampling technology in water and air.

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Sediment transfer and toxicity of novel halogenated disinfection byproducts of the pharmaceutical agent, gemfibrozil to marine organisms.

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Chlorination during wastewater treatment has been shown to be an effective practice for the removal of emerging contaminants. However, a negative feature associated with this method is the formation of halogenated byproducts that in many cases can be persistent and more toxic than the parent compounds targeted for removal. Halogenated byproducts of the pharmaceutical agent, gemfibrozil have been identified in several effluents from different wastewater facilities in Southern California USA. Assessment of the toxicity of these compounds have shown enhanced toxicity to polychaete worms (*Nereis arenaceodonta)* through both aqueous and sediment exposure. Aqueous exposure to fish have also shown enhanced anti-androgenic activities. These data suggest formation of novel chlorination byproducts from municipal and other water treatment activities such as desalination may increase the risks of discharge to the environment.

Emcon 2021

Modeling the fate of ionic pharmaceutical and personal care products (iPPCPs) in soil-plant systems: pH and speciation

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Abstract

A model was developed to simulate the pH-dependent speciation and fate of ionic pharmaceutical and personal care products (iPPCPs) in soils and their plant uptake during the application of reclaimed wastewater to agricultural soils. The simulation showed that pH plays an important role in regulating the plant uptake of iPPCPs. Four iPPCPs i.e., ibuprofen (IBU; with a carboxylic group), triclosan (TCS; phenolic group), fluoxetine (FXT; amine group), and tetracycline (TCL; phenolic groups and an amine group) were considered as model compounds. Under four different scenarios, it took 89 to 487 days for the iPPCPs to reach the steady-state concentrations in soil and plant tissues. The steady-state concentrations of iPPCPs in plant tissues at pH 9 is 2.2 – 2.3, 2.5 – 2.6, 1.07 – 1.08, and 6.6 – 6.9 times that at pH 5 for IBU, TCS, FXT, and TCL, respectively. Negating dissimilar sorption of neutral and ionic species or assuming sorption only for neutral species of iPPCPs led to miscalculation of iPPCPs concentrations in plant tissues by up to seven orders of magnitude. Efflux of compounds in soil, lettuce leaf, and soybean fruit was primarily contributed by their degradation in soil and dilution due to plant tissue growth. Overall, the results

demonstrate the importance of considering pH and speciation of iPPCPs when estimating their fate in the soil-plant system and plant uptake.

Characterisation and optimisation of novel bacterial laccases for the degradation of aromatic organic pollutants

Nabangshu Sharma, Ivanhoe KH Leung

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Persistent and emerging organic pollutants are toxic chemicals that are present in the environment including waterways and wastewater effluents. A significant portion of these pollutants are aromatic organic compounds, including but not limited to pharmaceuticals, endocrine disruptors, and industrial chemicals such as dyes, phthalates and bisphenols. These compounds possess a major threat to human health and the aquatic ecosystem.

The use of enzyme technology as a sustainable means for the degradation of water pollutants has gained considerable momentum in recent years. Laccases are versatile multi-copper oxidases that catalyse the oxidation of phenolic and aniline substrates. Thus, they offer the exciting prospect of sustainable treatment of aromatic water contaminants. My research focusses on the application of laccases as biocatalysts to degrade aromatic pollutants. In this talk, I will report my work on the characterisation and optimisation of two putative laccases from extremophilic bacteria. By using organic dyes as model compounds, the ability of these novel laccases to degrade aromatic pollutants was also explored. Finally, these enzymes were engineered though immobilisation technology to improve their operational stability and reusability. My work further demonstrates the potential of using oxidative enzymes such as laccases to break down toxic chemicals that possess major threats to human health and the environment.

Title: Targeted perfluorooctanesulfonate (PFOS) removal by spent coffee ground biochar modified with a PFOS molecularly imprinted polymer

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Abstract: Per- and polyfluoroalkyl substances (PFAS) are prevalent and persistent contaminants with demonstrated negative impacts to human and environmental health. Current PFAS separation technologies (i.e., activated carbon adsorption) lack selectivity, often necessitating pre-treatment of waters containing co-occurring contaminants which may be prohibitively expensive for facilities such as wastewater treatment plants (WWTP), which have been identified as important non-point sources of PFAS to aquatic systems. Molecularly imprinted polymers (MIPs) have been successfully designed for high adsorption selectivity of short and long chain PFAS. However, adoption of these materials in water treatment has been limited by poor performance at circumneutral pH and MIP immobilization requirements to improve retention. Biochar is an ideal MIP immobilization substrate because of its high specific surface area, ease of modification, and low production cost. This study describes the novel functionalization of a quaternary ammonium MIP onto coffee ground biochar (SCGKOH@MIP). First, biochar amine surface functional group density was increased via sequential aromatic electrophilic substitution and reduction. Amine groups functioned as binding sites for radical initiated polymerization of the perfluorooctanesulfonate (PFOS) imprinted MIP. Preliminary evaluation using simulated wastewater effluent showed highly selective PFOS removal, and the material demonstrated maintenance of a highly positive surface charge in environmental pH ranges – key for maintaining good PFAS adsorption. Regeneration tests showed good adsorbate recovery and high PFOS removal capability over multiple reuse cycles. SCGKOH@MIP represents a sustainable, cost effective water treatment alternative for targeted PFAS removal through reduced pretreatment requirements and increased material lifetime using low-resource regeneration methods.

Identification and Assessment of Emerging Contaminants in Drinking Water, Wastewater and Surface Water in Kampala, Uganda

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Kampala, the capital and the largest city of Uganda, is reported to be one of the fastest-growing cities in Africa with an estimated population of 1.5 million people as of 2019. The city resides on the northern shore of Lake Victoria, which is one of the largest lakes in the world. However, the rapidly growing population has created a challenge for the environment and public health. In Kampala, only around 60% of the population has a piped water supply. Around 35% of the population uses protected springs or unprotected springs as their drinking water sources. In addition, 54% of the wastewater is treated, while 46% of the wastewater is released. Therefore, the untreated or poorly treated wastewater could be a threat to drinking water resources and surface water, as it may contain a variety of emerging contaminants (ECs). The occurrence of ECs in drinking water, surface water, and wastewater in Kampala is still largely unknown. In this study, we collected 106 water samples from 34 sites including springs, wastewater treatment plants, and surface drainage channels in 2018 and 2019. We applied a suspect screening method using liquid chromatography-high-resolution mass spectrometry to screen for over 1627 ECs contained in an in-house database. We tentatively identified 355 ECs as suspect hits (detected at least once) in all samples. So far, we have confirmed 22 suspect ECs including 16 pharmaceuticals, 3 pesticides, and 3 personal care products. Ongoing work in our laboratory is focused on the confirmation and retrospective quantification of suspects.

Impact of widespread urban burning during the 2018 Camp Fire, California, on contaminants of emerging concerns in watershed

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Wildfire occurrence and intensity are increasing worldwide due to climate change. With increasing burning, destruction of wildland-urban interface communities during fire may cause contamination of surrounding waterways by ash and debris from burned structures, cars, and buildings. However, the effects of burned urban residues in surface water are not well understood in terms of contaminants of emerging concerns. In this study, we collected stormwater samples for one year following the November 2018 Camp Fire, the most destructive fire in California history with near 18,000 structures and thousands of vehicles burnt. We comprehensively characterized organic contaminant profiles and dynamics via targeted quantification of 35 stormwater-derived chemicals and complementary HRMS suspect screening. For quantified analytes, pentachlorophenol, a wood preservative pesticide and a likely human carcinogen, dominated the chemical profiles with concentrations up to 2400 ng/L and detection frequency of 89%. In one sampling site close to a burnt pharmacy, 6400 ng/L of ibuprofen and 1500 ng/L of caffeine was detected in November 2018, and suspect screening revealed acetaminophen and lidocaine presence in the same sample with rare detections of these pharmaceuticals in other locations. Suspect screening also revealed high levels of perfluorinated compounds in samples collected in November 2018 compared with those collected in the following year. These results highlighted the impact of urban burning on the release of contaminants of emerging concerns into surrounding watersheds, and identified potential threats to human and ecological health.

Towards a Tiered Approach to Assess Effects of Contaminant Mixtures in Urban Streams

Jonathan R. Behrens, Nishad Jayasundara, Emily S. Bernhardt,

Most efforts to measure contaminant concentrations and their biological effects in streams and rivers are limited to single points in time or single contaminant classes, rather than prevalent mixtures known to often be present. Further, it is cost prohibitive to monitor the large number of emerging and legacy contaminants (PFAS, PAHs, PPCPs, pesticides, micro and nanoplastics) found in most urban waterways or to determine the health outcomes of exposure to environmentally relevant mixtures. Thus, improving water quality requires: a) accounting for harmful biological effects of emerging and legacy chemicals when in mixture; b) identifying problematic contaminants and b) determining their primary sources. We propose a novel framework to rapidly and efficiently assess the effects of contaminant mixtures in urban streams, and potential sources. We will present a conceptual overview of a project underway in Ellerbe Creek, NC. The urban stream is composed of 36 sub-catchments; each vary widely in historic and current land use, population density, socioeconomic status, and the condition of their water infrastructure. Our approach will pair bioassays with targeted and non-targeted chemical analyses of water and biota samples to identify sub-catchments at highest risk of exposure to toxic contaminant mixtures. Bioassays will expose model organisms, zebrafish, to water samples from each sub-basin and assess the adverse biological outcomes of the contaminant exposure (i.e., development, growth, sub-cellular effects based on novel high-throughput assays). Targeted chemical analysis, of both water samples and a sentinel species (tetragnathid spiders), will quantify compounds indicative of individual pollutant sources (e.g. Sucralose for sewage, Glyphosate for lawns, Polybutadiene for road runoff). For sites of highest concern, non-targeted chemical analysis will be pursued to broadly characterize the contaminant mixture of water samples. The results will be a first estimate of the effects of contaminant mixtures, at environmentally relevant conditions, for the highly urbanized stream in Durham, NC. This tiered approach can speed discovery of harmful contaminant mixtures and assess the potential for bioaccumulation and harmful ecotoxicological effects.

Title: Towards Predictive Models for Virus Inactivation by Chlorine

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Characterizing the factors that influence viral inactivation in engineered systems is essential to protect public health from emerging viral contaminants and comply with pathogen regulations. Chlorine is a widely used disinfectant in water and wastewater treatment, but it is difficult to predict chlorine reaction kinetics with non-culturable and emerging viruses, as chlorine susceptibility can differ widely across and within viral classes and families. Additionally, wide variation in methodology of viral inactivation studies challenges broad data interpretation and clouds our ability to pinpoint future research needs. To clarify the significance of existing data and identify data gaps, we conducted a systematic review of 1300 papers on chlorine inactivation of viruses. Abstracts and titles were organized using Rayyan software and scanned for relevance by two reviewers. The full texts of 460 articles passing this stage were subsequently reviewed. Papers were included if they quantified inactivation using a culture-based method, used chlorine concentrations and time points relevant to water treatment, and quantified chlorine decay throughout the experiment. First or second-order rate constants for reactions with chlorine were extracted and grouped by virus class and family, and gaps in the inactivation literature were identified. When multiple rate constants were extracted for a single virus, a single rate constant was calculated based on the data. In this presentation, the results of the systematic review will be discussed as will the efforts to predict inactivation of emerging viruses. The findings of this study will clarify the selection of appropriate surrogates for human viruses in chlorine disinfection systems.

Becky Curtis: Abstract for poster presentation, EMCON21

Title: Copper phosphate nanosheets as an agrofertilizer: implications for environmental behavior, transformation, risk towards aquatic species

Authors

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Abstract

Nanomaterials contribute to innovative applications across numerous industries due to specifically engineered characteristics such as size, shape, and surface functionalization. The superior efficacy of nano-enabled agrochemicals compared to their bulk-formulated counterparts may allow improved agricultural production while reducing chemical inputs. However, direct application to agricultural environments introduces the possibility of both terrestrial impacts and nanomaterial entry to aquatic systems through runoff and subsequent biological impacts towards aquatic species. Regarding the use of these nanomaterials, there is a need to further understand both the potential risks and the possibility for the mitigation of environmental degradation posed by agricultural activities. The current work examines nano-copper phosphate ($Cu_3(PO_4)_2$) as an agrofertilizer and seeks to better understand potential impacts by investigating differences in environmental deposition and transport through soil matrices between these nanomaterials and other agrochemicals formulated with bulk or nano copper. Interactions between the various chemicals and soil are assessed through the simulation of runoff, which is analyzed for levels of copper found in particulate vs. water fractions to assess potential threats to benthic- vs. pelagic-dwelling species. To further understand consequences of exposure of aquatic species to environmentally relevant exposure scenarios, the current work also evaluates the transformation of $Cu_3(PO_4)_2$ particles occurring after interaction with field runoff. Findings of this work will inform sustainable use of nano-$Cu_3(PO_4)_2$ in the agricultural sector and enhance predictive capabilities for potential impacts to aquatic species.

Environmental assessment of heavy metals contamination of soil in selected dumpsites in Niger delta, Nigeria.

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Abstract

In this investigation, the level of heavy metals (Zinc, Manganese, Cadmium, Copper, and Lead) was determined using Atomic Absorption Spectroscopy in sediment samples from dumpsite locations in Warri, Delta State, Nigeria. The potential contamination and toxicity of studied metals were determined by evaluating the Contamination Factor (CF), Geo- accumulation Index(Igeo) , ecological risk assessment (ERA), Pollution Load Index(PLI), and Hazard Index(HI). Considering spatial distribution patterns, metal concentrations were lower than the WHO/FAO and Dutch standard permissible limits in all samples, except for Zinc in Osubi Abattoir dumpsite. In this study, Contamination Factor and Geo- accumulation Index values revealed that sediments were moderately polluted by Lead and Zinc in three (3) locations and unpolluted by other metals. The evaluation of the ERA based on the Contamination Factor (CF), Geo- accumulation Index(Igeo) , ecological risk assessment (ERA), Pollution Load Index(PLI), and Hazard Index(HI) revealed that the sediments show no sign of pollution, except in location 9, whose value of 0.91 was very close to the baseline value of 1, signifying incoming pollution and generally low risk except for lead, which shows low moderate risk. The strong positive association between Lead/Copper, Manganese / Copper, and Zinc/Manganese based on Pearson's correlation coefficient, suggests a similar source.

Assessing Haloacetonitrile Formation from Model Nitrogenous Precursors

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Disinfection byproducts (DBPs) are chemicals of concern in drinking water, many of which arise from the reactions between organic matter and disinfectants. Only a small number of DBPs are regulated by the United States Environmental Protection Agency. Among the broad range of DBPs that remain unregulated, haloacetonitriles (HANs) emerge as a high priority DBP class due to their high toxicity and occurrence in drinking water. HANs are formed during chlorination from nitrogenous precursors such as amino acids prevalent in algal and wastewater-impacted waters. This research employs model precursors to investigate the formation mechanisms of chlorinated and brominated haloacetonitriles (*i.e.*, dichloroacetonitrile (DCAN) and dibromoacetonitrile (DBAN)) during free chlorination and free bromination, respectively. Tryptophan (Trp) and two of its derivatives, *N*-acetyltryptophan (NAT) and 3-indolepropionic acid (IPA), were utilized as model precursors. Among these three precursors, tryptophan exhibited the highest HAN formation under both chlorination and bromination conditions. Less, but not negligible, HAN formation was observed for both NAT and IPA. For example, after 3 hr, Trp, NAT, and IPA formed 446, 204, and 51 nM DCAN, and 543, 457, and 58 nM DBAN, respectively. These results show that at timescales relevant to water disinfection practices, bromination yielded higher concentrations of DBPs, and suggest that the indole moiety in Trp can contribute to HAN formation. The latter is a noteworthy finding as most of the current understanding of HAN formation focuses on free amino acids. Overall, our findings indicate a further need to understand the formation of HANs.

Age matters? Examining age-specific behavior and proteomic responses of zebrafish (*Danio rerio*) to a model toxicant

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Chemical safety data for industrial and consumer chemicals is necessary to characterize and manage risks to public health and the environment, yet is deficient for the vast majority of existing chemicals. These deficiencies, coupled with the significant time and monetary costs of traditional toxicity testing, have prompted a shift away from historically used methods towards those that reduce the number of animals, leverage existing data, and implement high throughput screening (HTS) techniques including the fish embryo toxicity test (FET). Whereas the FET test typically exhibits correlation with traditional Acute Fish Toxicity test (AFT) results, differences emerge between FET and AFT for some compounds and sublethal responses. Previous research in our lab reported that larval fish exposed to the antihistamine diphenhydramine (DPH) demonstrate increased mortality, uptake, and behavioral toxicity than their embryonic counterparts. However, whether dispositional factors and/or molecular initiation events influenced such age-specific differences were not defined. In the current research, we examined changes in the proteome of zebrafish exposed to DPH at sublethal concentrations during separate experimetns performed across embryonic, larval, juvenile, and adult life stages. Over 3200 proteins were identified and grouped based on gene ontology resulting in differential expression of proteins implicated in morphogenesis, angiogenesis, and neural development. By contrasting changes in whole-body protein expression with chemical exposure across age groups, we identified age and exposure-specific differences in the identity, proportion, and function of identified proteins.

Use of UV-LED based halogen advanced oxidation processes for removal micro-pollutants from DOM-rich bioreactor effluent

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UV-driven advanced oxidation processes (AOPs) provide a modern solution for the removal of emerging contaminants, such as pharmaceuticals, from wastewater treatment plant effluent. Here, hypochlorite photolysis is employed for the removal of four pharmaceuticals: Carbamazepine, Acetaminophen, Tetracycline, and Sulfamethoxazole. The UV/chlorine AOP works via the production of reactive oxygen and chlorine species (ROS and RCS). The presence of RCS is advantageous for DOM-rich effluent due to their selectivity and affinity towards aromatic compounds. UV-LEDs provide further advantage over traditional Hg-fluorescence approach given their higher molar absorptivities at newly available UV wavelengths at relevant pH values. This study analyzes the performance of the UV/chlorine system over a variety of conditions including pH, chlorine content, DOM concentration and DOM-type. THE UV/chlorine system is also compared with the UV/H_2O_2 system for efficiency. An EPR analysis was conducted to identify and study the role of RCS vis-à-vis ROS in the system.

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Computational approaches for the prediction of environmental transformation products: Chlorination of steroidal enones

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ABSTRACT

There is growing interest in the fate and effects of transformation products generated from emerging pollutant classes, and new tools that help predict those products most likely to form will aid risk assessment. Here, using a family of structurally related steroids (enones, dienones, and trienones), we evaluate the use of density functional theory (DFT) to help predict products from reaction with free chlorine, a common chemical disinfectant. For steroidal dienones (e.g., dienogest) and trienones (e.g., 17β-trenbolone), computational data support that reactions proceed through spontaneous C4 chlorination. This yields near exclusive 4-chloro derivatives for trienones whereas further reaction of dienones yields 9,10-epoxide structures. For testosterone, a simple steroidal enone, *in silico* predictions suggest that C4 chlorination is still mostly likely but slow at environmentally relevant conditions. Predictions were then assessed through laboratory chlorination reactions (0.5-5 mg Cl_2/L) with product characterization via LC-HRMS and NMR, which confirmed major 4-chloro and 9,10-epoxide products for trienones and dienones, respectively. Also consistent with computational expectations, testosterone was effectively unreactive at these same chlorine levels, although products consistent with *in silico* predictions were observed at higher concentrations (in excess of 500 mg Cl_2/L). Although slight deviations from *in silico* predictions were observed for steroids with electron-rich substituents (e.g., altrenogest), this work highlights the potential for computational approaches to improve our understanding of transformation products generated from emerging pollutant classes.

Quantitatively measuring freely dissolved cyanotoxins with diffusive gradients in thin films (DGT) samplers in recreational lakes of Southern California, USA

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Cyanotoxins can be extensively generated by harmful algal blooms and are highly toxic to aquatic life. To properly estimate the risk of cyanotoxins in the ambient environment, quantitative measurement of their freely dissolved, i.e., bioavailable, concentrations becomes an emerging demand. The diffusive gradients in thin films (DGT) sampler have been applied to measure some microcystin variants. However, lack of reliable diffusion coefficient (*D*) values is a bottleneck to apply the DGT sampler for more cyanotoxins. The goal of the present study was to develop a passive sampling method with DGT samplers for cyanotoxins, particularly for non-microcystin compounds. In this work, diffusion coefficient (*D*) of microcystins, cylindrospermopsin and anatoxin-a in polyacrylamide gel (PA gel) were measured using a stack method. The effect of temperature on diffusion was investigated via measurements at 4, 15, and 25 °C. DGT samplers with the PA gel as diffusive gel and agarose-HLB gel as binding gel were deployed in several recreational lakes in southern California to determine cyanotoxin levels. Several microcystin congeners were detected in the lakes and quantified with the laboratory-measured *D* values. This work demonstrated that the DGT sampler is an effective tool for monitoring cyanotoxins in the environment.

Title: Evaluating permeable pavements as a stormwater management technology for tire wear particle attenuation

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As tires wear on roads, they generate rubber microplastics which are now ubiquitous in stormwater and aquatic environments. Tire wear particles (TWPs) leach 6PPD-quinone which has been identified as the causal toxicant for Urban Runoff Mortality Syndrome (URMS) in coho salmon. Given the ubiquity and toxicity of TWPs and their leachable contaminants, there is an imminent need for stormwater management practices that attenuate TWPs and prevent release of 6PPD-quinone into surface waters. Permeable pavements (PPs) are an established stormwater management technology which allows water to infiltrate rather than runoff of paved surfaces. PPs remove particulate matter from stormwater, suggesting that they may also be capable of trapping TWPs. Since PPs are periodically unclogged by vacuum sweeping, TWPs retained in the pavements may be disposed of during maintenance. However, trapping of TWPs in PPs may introduce the risk that 6PPD-quinone could leach from retained particles during subsequent storms. A bench scale study is being carried out to estimate TWP retention in permeable pavements, and to assess the risk of 6PPD-quinone leaching from trapped TWPs. TWPs (cryomilled, 50µm) will be deposited on the surface of PP cores, and the cores will be dosed with clean water to simulate deposition and infiltration of TWPs into PPs. A mass balance will be conducted of particles deposited on the cores and recovered in the effluent to estimate the TWP trapping efficiency. 6PPD-quinone will be measured in the effluent using GC/MS to estimate leaching within the pavement. Subsequent clean water applications will be used to estimate the duration of TWP and 6PPD-quinone release following deposition.

EMCON Poster

Engineering application of soluble biochar for pollutant removal

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Engineering application of biochar for water treatment has attracted a great deal of interest due to its low cost and special reactivity. Our recent study showed that the aqueous (soluble) biochar can be reactive toward the degradation of organohalogen. However, barriers exist for the engineering application of soluble biochar toward treatment of wastewater or remediation of polluted groundwater aquifers. This study targets to investigate the solutions enabling the pilot-scale application of soluble biochar. First, the biochar has been re-reduced after reaction with organohalogen (using triclosan (TCS) as a model compound) and reacted with TCS again. Our results indicate that the electron donating capacity of soluble biochar is almost fully recyclable. The pseudo-first order reaction rate constant between soluble biochar and TCS was very similar for that re-reduced compared to the original material. Second, multiple ways have been explored for extraction of soluble biochar from the bulk materials, including sonication, organic solvent extraction, and ozonation-extraction. Extracted soluble biochar will be characterized for their composition using mass spectrometry, reactivity including electron donating capacity, and reaction rate constant with model organohalogen. The comparison is expected to provide insights into the best way to extract a good amount of soluble reactive components from bulk biochar. Expected results from this work will lay the foundation to scale up the application of soluble biochar to degrade organic pollutants for wastewater treatment or groundwater aquifer remediation.

POSTER ABSTRACTS

Emcon: International Conference on Emerging Contaminants

September 13–14, 2021

Virtual Event Hosted by University of Washington

ABSTRACT BY CHIGBO ADAEZE RUTH

TITLE: SUITABILITY OF LATERITIC SOIL FOR ROAD CONSTRUCTION A MEANS CARBO SEQUESTRATION AND ENERGY MANAGEMENT

This work was carried out to investigate the innovation of cost effective model for energy management ensuring a sustainable environment. When fossil fuel burns, carbon dioxide is emitted leading to increase in global warming. Geotechnical investigations were carried out to determine the textural and structural properties of the soil as it relates to its stability to road construction and ability to absorb carbon dioxide. Samples were collected from 6 locations in Delta and Enugu States. In accordance with AASHTO classification scheme, results showed that liquid limit ranged from 18% to 36%, plastic limit varied from 13.15% to 24% while plastic index is between 8.9% and 17.6%, the optimum moisture content varied from 10.30% to 24.3%. The evaluation reveals that the lateritic soils have lower plastic index and optimum moisture content. This reviews that lateritic soil that is of A-3, A-2-7, A-1 and dominantly A-2-4 does not deteriorate fast when used as road pavement material. Research showed that Olivine when added to the soil can improve soil mechanical properties and also sequester carbon dioxide from the surrounding environment. Moreover use of organo-metallic compounds as additive to reduce carbon dioxide emitted by vehicle was analyzed. Improving the ability of the asphalt to absorb Carbon dioxide should be considered by Geoscientist and road workers. More avenues should be provided for further studies on this topic as it will serves as a future prospect for energy management ensuring safe environment, a base line in enhancing Geosciences education.

KEYWORDS: Carbon emissions, lateritic soil, geotechnical properties, Classification and Atterberg limit

UNSCHEDULED ABSTRACTS

Emcon: International Conference on Emerging Contaminants

September 13–14, 2021

Virtual Event Hosted by University of Washington

Title: A liquid chromatography tandem mass spectrometry method for the quantification of selective analgesics and their metabolites in wastewater influent

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Abstract

Wastewater-based epidemiology (WBE) is an established tool to analyse patterns of community drug use. In recent times, monitoring the use of analgesics has become a public health priority. An analytical method was developed, optimised and validated for a broad range of common analgesics (non-steroidal anti-inflammatories and opioids) and their metabolites at trace concentrations in wastewater influent. Samples were analysed via liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) with an electrospray ionization source (ESI) in both positive and negative ion multiple reaction monitoring modes. Fifteen of the thirty-five biomarkers were validated for LC-MS/MS analysis by direct injection, while the other 20 biomarkers were present in wastewater at lower concentrations, requiring extraction by solid phase extraction (SPE) using Oasis HLB cartridges. The limit of quantification (LOQ) ranged between 17 ng/L - 191 ng/L and 13 ng/L -110 ng/L for direct injection and SPE, respectively. Recoveries for SPE ranged between 80% and 120%. Following validation, the method was applied to 28 wastewater samples from four municipal wastewater treatment plants. Twenty-eight of the thirty-five analgesic biomarkers were detected in the samples at concentrations of between 0.03 and 289 µg/L. Population normalised mass loads ranged from 10 mg/day/1000 (meperidine) to 72,000 mg/day/1000 (paracetamol) among all investigated compounds. The described method is a suitable analytical tool for wastewater-based epidemiology applications to estimate analgesics consumption.

PFAS in Nevada water systems: occurrence, treatment, bioaccumulation, and interaction with microplastics

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Critical data gaps exist in PFAS occurrence, sources, and fate and transport in the Nevada water systems. In southern Nevada, treated wastewater is a valuable water source but it also introduces toxic chemicals to the primary water supply reservoir, Lake Mead. Given the water scarcity in southern Nevada during the exceptional drought in 2021, PFAS can concentrate in the water system to increase bioaccumulation potentials and put pressure on water treatment. This presentation summarizes the up-to-date research efforts on PFAS in the southern Nevada watersheds, including the occurrence and distribution in surface water and sediments, mass balance during municipal wastewater treatment processes, and fate and transport studies. This study evaluated the bioaccumulation and uptake of PFAS by the freshwater green algae *Nannochloris* and *Chlorellar*. The results provide insights into the food web transfer of PFAS in aquatic ecosystems as well as potential application of using algal ponds to remove PFAS. In addition, the interaction between PFAS and polyethylene microbeads (i.e., 50 µm vs. 150 µm) was studied in sediment-water systems.

Watershed-Scale Integrated Ecotoxicological Assessment: Implications of Exposure to Complex Inorganic and Organic Chemical Mixtures

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River waters intrinsically contain complex mixtures of inorganic and organic constituents derived from natural and anthropogenic sources. Aquatic organisms exposed to these heterogenous matrices may experience potential mixture effects, which can have cascading ecosystem consequences. Concurrent assessment of landscape, hydrological, chemical, and biological variables was applied to the Shenandoah River Watershed (USA) to develop a holistic understanding of complex interactions between sources, exposures, and effects. On-site mobile laboratory experiments were conducted to evaluate apical and molecular effects on fathead minnows (*Pimephales promelas*) from chemical mixture exposures. A total of 534 constituents were measured, including inorganic (nutrients, major ions, and trace elements) and organic (pesticides, pharmaceuticals, personal-care products, industrial chemicals, disinfection byproducts, and per- and polyfluoroalkyl substances) compounds, of which 273 were detected in the 56 samples analyzed (concentrations ranged from $<1.0\times10^{-4}$ to 4.7×10^{4} $\mu g\ L^{-1}$ and detection frequency ranged from 2 to 100%). A municipal wastewater reuse model was developed to predict concentrations of constituents derived from wastewater treatment-plant discharges for 1,754 stream reaches in the Shenandoah River watershed. Measured and modeled environmental concentrations generally were within a factor of 2. The wastewater-reuse model output was used to predict aquatic organism exposure to chemical mixtures and evaluate potential biological effects. Risk quotients (RQs) were calculated for individual constituents in the mixture and the majority had values <0.1 (indicating limited risk). However, when individual RQs were summed to give an additive risk index (RI), aggregated chemical stressors from municipal wastewater pose widespread potential risk (RI values >10) to aquatic organisms.

Pharmaceuticals and Contaminants of Emerging Concern in Washington's Wastewater: Ecology's Prioritization and Mitigation Strategy

Frances Bothfeld, CEC Policy Coordinator, Washington State Department of Ecology, Water Quality

Pharmaceuticals, personal care products (PPCPs), and other contaminants of emerging concern (CECs) enter Washington's state waters through wastewater treatment plants (WWTP). The bioaccumulative effects of these contaminants can have damaging effects on aquatic life, especially apex predators like the Southern Resident Orca Whale Population. The Washington State Legislature and the Governor's office requested Washington's Department of Ecology to investigate how to limit PPCPs and CECs from wastewater effluent. Over the next few years Ecology aims to prioritize contaminants of emerging concern, investigate source control alternatives, review different wastewater treatment technologies, and create recommendations to reduce CEC loading into surface waters.

The first two goals are to identify and prioritize a suite of CECs for monitoring and to develop management responses based on biological relevance. This information is critical to prioritize the limited resources to address the chemicals of greatest concern. Ecology's other goal is to develop a directory of treatment technologies that includes removal rates for the priority suite of CECs. Ecology just released a paper that reviews different wastewater treatment technologies. This directory provides information on the ancillary benefit of CEC removal from nutrient removal treatment processes. With this information, Ecology can begin to determine how to address competing regulatory priorities and reduce CECs entering the environment.

Conference: EMCON2021

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Regulated and Emerging Contaminants in Tapwater: Point-of-Use Mixture Exposures and Potential Effects Screening

Paul M. Bradley, Kristin M. Romanok, Kelly L. Smalling, Michael J. Focazio, Dana W. Kolpin

The magnitudes, cumulative dose-response relations, and potential adverse outcomes of drinking-water exposures to complex mixtures of regulated and emerging-concern contaminants are global research priorities. Target assessments of mixtures of inorganic and organic contaminants in point-of-use drinking water (tapwater) are being conducted to inform tapwater exposures and corresponding estimations of cumulative human-health risks across the US. More than 460 organic, 35 inorganic, and select microbiological contaminant indicators are assessed in tapwater from home and commercial locations supplied by federally-regulated public community water systems and federally-unregulated private-wells. Analytical results demonstrate that human exposures to inorganic and organic contaminant mixtures, which are rarely monitored together in drinking water at the point of consumption, are common. Concentrations of regulated and unregulated TW contaminants are used to calculate cumulative *in vitro* bioactivity ratios and Hazard Indices (HI) based on existing human-health benchmarks. Exceedances of human-health benchmarks and health-based HI screening levels of human-health interest are common to both public and private drinking water supplies. Study findings support further investigation of the potential cumulative risk to vulnerable populations and illustrate the importance of continued broad characterization of tapwater exposures using analytical capabilities that better represent the documented complexity of contaminant mixtures in ambient source waters.

Microplastic Pollution in California: Using Scientific Guidance to Inform a Precautionary Framework that Assesses and Addresses Risks to Marine Ecosystems

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Keywords: microplastic, risk prioritization, marine ecosystems, persistent pollutant, fate, transport, occurrence, priority species, source reduction

In 2020, a group of experts was convened by the California Ocean Science Trust to assess the state of the science in the field of marine microplastics and construct a framework that would accurately assess potential risks to marine ecosystems in California. The group of toxicologists, ecologists, chemists and risk assessors drawn from academic, government, and private sectors were also charged with providing concrete actions to be taken in light of threats to resident marine species and habitats. Following several months of work and consideration, key recommendations arising from this process were that California should use a precautionary approach to assess and manage microplastic pollution risk, because there are realistically no feasible cleanup options for this persistant pollutant, and because projections point to a predicted increase in environmental concentrations. The current body of knowledge in the greater field strongly suggests that microplastics can lead to adverse effects in organisms and humans. High priority components of the framework and risk prioritization tool developed from the group include a) consideration of certain particle morphologies and polymer types (e.g., fibers, tire wear particles), b) specific fate and transport pathways such as stormwater runoff and aerial deposition, c) characterizing sources in the state (e.g. tire and road wear, laundry / textiles), and d) an emphasis on priority endpoints that constitute taxonomic groups of highest concern, both ecologically and in terms of importance as fisheries (e.g. mollusks, crustaceans, fish). This presentation will describe the risk prioritization tool that was developed and recommended source reduction strategies and data gaps that were highlighted by the working group. Future steps concerning California's plan for reducing plastic pollution and supporting data collection efforts to increase the existing knowledge base over the next five years will also be described. The broad recommendations issued in this report represent the first such effort in the United States, and thus progress made since the report was published, in both legislative and research arenas will also be highlighted.

Modified Biochar for Sorptive Removal of Emerging Contaminant

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Pharmaceuticals cured deadly diseases and enhances life spans of human beings. But, in the past decade, pharmaceuticals have risen as a “contaminant of emerging concern” around the world. The persistence and resistance of pharmaceuticals leads to their accumulation in water bodies. Inefficiency of conventional WWTPs to remove pharmaceuticals also contributed to their environmental presence. Thus, urgent need of sustainable and economically feasible remediation techniques has become evident. The present study describes the sorption of Acetaminophen from aqueous systems with modified biochar. The modified biochar was developed from Mg/Al layered double hydroxides impregnated rice husk biomass at 500 and 700 °C in an atmosphere-controlled muffle furnace. The developed modified biochar was characterized by CHNS analyzer, ICP-OES, SEM, SEM-EDX, TEM, FTIR, and XRD. Modified biochar was applied for aqueous pharmaceutical removal in batch mode through pH, isotherm and kinetic studies. The effect of pyrolysis temperature, pH, concentration, dose, contact time, and sorption temperature have been evaluated. Modified biochar prepared at 700 °C shows significantly higher removal of pharmaceutical as compared to modified biochar prepared at 500 °C as well as pristine biochars.

Keywords: Pharmaceuticals, Adsorption, Biochar-Layered double hydroxides.

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Title: Halogen Radicals Contribute to the Halogenation Chemical Additives in Hydraulic Fracturing Fluids

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Abstract:

In hydraulic fracturing (HF) fluids, halogenated transformation products have been identified as emerging contaminants. The formation of halogenated contaminants may result from the use of the breaker persulfate. Persulfate generates sulfate radicals that are scavenged by high concentrations of halides in HF fluids, producing halogen radicals (e.g., $Cl^{\bullet}$, $Br^{\bullet}$, $Cl_2^{\bullet-}$, $BrCl^{\bullet-}$, $Br_2^{\bullet-}$). Because halogen radicals have been implicated in the formation of halogenated contaminants in advanced oxidation processes, we hypothesized that halogen radicals are responsible for the formation of halogenated contaminants in HF fluids. In this study, we demonstrate that halogen radicals lead to the halogenation of organic additives used in HF fluids. We first found the formation of halogenated products of organic additives cinnamaldehyde (i.e., α-chlorocinnamaldehyde and α-bromocinnamaldehyde) and citrate (i.e., trihalomethanes) under typical HF conditions (e.g., 80 °C, pH 7). Next, we found that the addition of isopropanol as a radical quencher reduced the production of these halogenated products to levels below their detectable limits, indicating that halogen radicals are the key intermediates in the halogenation of cinnamaldehyde and citrate. Our results in overall demonstrate that halogen radicals contribute to the formation of halogenated contaminants in supersaline subsurface HF fluids.

Title: **Evaluating pesticide application data to determine the drivers of aquatic pesticide pollution in the Western Cape, South Africa**

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Abstract

Agriculture is an essential sector to South Africa's economy, which has made it the leading user of pesticides in Sub-Saharan Africa. Consequently, there is an urgent need to better understand how pesticides could be entering non-target environments, particularly water where it could potentially affect aquatic ecosystems and human health.

Our current research evaluates datasets from three sampling campaigns in the rivers of three agricultural catchments (i.e., Grabouw, Hex River Valley, and Piketberg) within the Western Cape, South Africa. The sampling campaigns were conducted over three years: 2017 (July to December); 2018 (January to June) and 2019 (April to July) using passive water samplers. Additionally, pesticide application records were collected over the same periods.

By evaluating these datasets, we have gained a better understanding of why specific pesticides are being detected while others are not. We have compared the levels of aquatic pesticide pollution to Environmental Quality Standards (EQS) to gauge its severity. We found that eight pesticides have exceeded EQS values in at least one of the sampling campaigns. Imidacloprid is of particular concern because it has consistently exceeded EQS values in all three years. Additionally, fungicides were found to have been applied in the highest quantities yet were detected the least. This may be partially due to their chemical properties (i.e., short half-life and high sorption). Our research showcases methods to sample and evaluate data from longitudinal water monitoring for pesticides along intensive agriculture systems in a middle-income country.

Detrimental effects of tire wear particles and leachate on model organisms *Danio rerio* and *Daphnia magna*

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Annual production of plastics has grown to several hundred million tons. Environmental sampling has found a diversity of plastic types including high levels of black rubber. Tire wear particles (TWPs) originate from friction of tires on roads. The impact of this flow of TWPs to the environment is not known. Available literature focuses on the toxicity of leachate, overlooking potential effects of the TWPs. We conducted experiments to assess particle and chemical toxicity of micro (1-20µm) and nano (<1µm) TWPs to model organisms, *Danio rerio* and *Daphnia magna*. To assess effects on development, zebrafish embryos were exposed to concentrations ranging from 1.0 x 10^3 to 3.0 x 10^9 particles/ml (n=18, four replicates). In embryonic zebrafish, high concentrations of all exposures significantly decreased spontaneous movement at 24 hpf. Greater toxicity was observed following nano TWP and leachate exposure as compared to micro TWPs. This is some of the first research to show that exposure of zebrafish to nano TWPs, has detrimental effects. We observed *D. magna* mortality following a 48 hour exposure of neonate, ranging from 1.3 x 10^5 to 3.3 x 10^9 particles/ml (n=15, three replicates). LC_{50} calculated for micro and nano TWPs were 4.7 x 10^5 and 3.0 x 10^8, respectively. Much of the particle mortality is explained by toxicity of the leachate. Overall, these aquatic species appear differentially susceptible to TWPs. It is important to identify the differing toxicities of TWPs to achieve an understanding of the impacts they have on an ecological community as a whole.

Title:

Quantification and spatial distribution of pharmaceuticals, personal care products, and perfluoroalkyl substances in Puget Sound sediments from 2010 through 2019.

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Abstract:

Pharmaceuticals and personal care products (PPCPs) and perfluoroalkyl substances (PFASs) are identified as chemicals of emerging concern (CECs) in Puget Sound, WA, due to their potential to cause adverse toxicological, biological, and ecological effects when unintentionally discharged to the environment. Characterization of sources, transport patterns, and the fate of CECs in the environment has been prioritized as part of the toxics monitoring strategy for the Sound. PFASs are also the focus of a 2021 Chemical Action Plan developed by the Washington State Dept. of Ecology (Ecology). Concentrations of PPCPs and PFASs have been measured and detected in influent, effluent, and biosolids from municipal wastewater treatment plants; in the tissue of invertebrates, fish, birds, and mammals in Washington State and in the Puget Sound watershed. For our survey, surface sediments from 50 Puget Sound-wide monitoring stations and six urban bays were sampled from 2010 through 2019. Analyses were conducted for PPCPs and PFASs by SGS-AXYS Analytical Services Ltd., Sidney, BC, Canada, using AXYS Method MLA-075, based on EPA 1694 and MLA-041, respectively. These methods use liquid chromatography coupled with tandem mass spectrometry (LC/MS/MS). Ecology's Manchester Environmental Lab also conducted PFAS analyses for these surveys. Results are summarized and presented graphically to indicate the concentration and distribution of PPCPs and PFASs in these Puget Sound sediments, with comparisons made among surveys.

Mathematical model development and calibration for microplastic reduction using hydrolytic enzymes

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Microplastics (MPs) are emerging contaminants that can cause serious problems in the aquatic environment and negatively affect the public health. MPs are small plastic particles that are less than 5 mm in size, including polyester and acrylic fibers from synthetic fabrics and microbeads from personal care products (e.g., toothpastes). Although membrane disc-filters and rapid sand filtration technologies can be used for MP removal during wastewater and sludge treatment processes, there are many challenges, such as: membrane clogging and potential bypass of small MPs through the filter grains, in implementing these technologies on large scale MP removal applications. Therefore, MP removal is limited in the conventional biological wastewater treatment processes. In this study, lab-scale experiments were conducted to investigate the reduction of polyethylene MP using hydrolytic enzymes (i.e., lipase, cellulase and protease) under mesophilic (37.5°C) and thermophilic (55°C) conditions at enzyme concentration of 22, 44 and 88 mg/L. Based on the experimental results, protease was the most effective enzyme on MP reduction. Moreover, the thermophilic temperature and high enzyme concentration enhanced the MP reduction. Beside the lab-scale experimentation, a non-steady state mathematical model was developed and calibrated using the experimental results to estimate the model kinetic constants for the three examined enzymes under mesophilic and thermophilic conditions. In conclusion, hydrolytic enzymes are effective on MP reduction, reflecting meaningful removal in anaerobic

digesters where hydrolytic enzymes are abundant from fermentative microorganisms. Also, mathematical model simulation results were essential to enhance our understanding of MP removal mechanisms and determine the dominant operational parameters on the MP reduction in wastewater treatment processes.

Toxicity of Novel Tire-derived Chemical 6PPD-quinone to Coho Salmon (*Oncorhynchus kisutch*) under Varying Environmental Conditions

Garrett Foster, Jill Wetzel, Ed Kolodziej, Jenifer McIntyre

Coho salmon (*Oncorhynchus kisutch*) returning to spawn in urban-impacted watersheds of the Pacific Northwest of North America suffer high rates of mortality from exposure to stormwater runoff. Juvenile coho salmon can serve as a surrogate for studying the observed mortality on adult spawners. Using juvenile coho, we recently identified a novel tire-derived chemical (6PPD-quinone) as the primary contaminant in roadway runoff responsible the acute mortality. Acute lethality was determined to be on the order of <1 µg/L under standard laboratory rearing conditions for juvenile coho salmon. Previous exposures were conducted under static 24-h conditions. Conditions in streams often differ from those in the laboratory, including differences in flow, temperature, and water chemistry. Many of these differences can affect the bioavailability and/or toxicity of chemical contaminants. To extrapolate lab-derived toxicity data for 6PPD-quinone to expected toxicity in the field, we will determine toxicity to juvenile coho under varying water quality (e.g., temperature, pH, ionic strength, dissolved organic matter) and flow conditions. This data will help elucidate what receiving water conditions result in maximal concentrations of bioavailable toxicant and put further at risk coho salmon and other vulnerable aquatic organisms.

The First Statewide Assessment of Antibiotic-Resistant Bacteria and Antibiotic-Resistance Genes in Iowa's Streams

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Widespread occurrence of antibiotics in Iowa's streams combined with the detection of elevated concentrations of antibiotic resistant bacteria (ARB) and presence of antibiotic resistance genes (ARGs) suggest that current agricultural practices are a source of antibiotic resistance to Iowa's streams through varied pathways (e.g. runoff and tile drainage). In 2019, the U.S. Geological Survey and the University of Iowa Center for Health Effects of Environmental Contamination completed the first statewide assessment of ARB and ARGs in water and bed sediment collected from Iowa streams. Sites were selected based on livestock production density and point source influence. Samples were plated on media for *Escherichia coli* and antibiotic-resistant *E. coli*, enterococci and antibiotic-resistant enterococci, and staphylococci and antibiotic-resistant staphylococci. Of the 34 water samples collected, 14 (41%) yielded Extended Spectrum Beta-Lactamase (ESBL)-producing *E. coli* growth, 2 (5.9%) had carbapenemase-producing *E. coli* growth¸ 30 (88%) produced vancomycin-resistant enterococci growth, and 18 (53%) were positive for resistant staphylococci growth. Of the 32 sediment samples, 7 (22%) yielded ESBL-producing *E. coli* growth, 5 (16%) had carbapenemase-producing *E. coli* growth¸ and (44 %) were positive for resistant staphylococci growth. DNA from growth was used in PCR assays targeting ARGs that encode resistance to antibiotics of clinical importance to human health and disease prevention and thus, their presence in streams could be of environmental significance. Results will provide a baseline understanding of ARB and ARGs prevalence throughout Iowa's waterways and health risk potential for humans, wildlife, and livestock using these waterways for drinking, irrigating, or recreating.

Characterisation of the chemical contents of per and polyfluoro substances in aquatic environmental systems using non-target screening and passive sampling technique

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Per- and polyfluoroalkyl substances (PFASs) are persistent environmental contaminants with over 5000 types estimated to be used in various formulations on the global market. Targeted methods of monitoring PFASs are not sufficient to characterise the new sources of PFAS. However, non-target screening is a powerful tool for discovery of PFAS.

Sampling technique plays an important role in the collection of representative samples. Grab sampling techniques only show a snapshot of the samples whereas passive sampling techniques could provide the time integrated concentration estimation over extended periods. Passive sampling techniques are also cost effective and can detect lower concentration of compounds.

In this study, non-target screening of PFAS was conducted using quadrupole time-of-flight tandem mass spectrometry (QTOF-MS) to discover PFASs in 15 aquatic environmental sources from nine countries including Germany, Austria, Slovakia, Serbia, Romania, Ukraine, Australia, The Netherlands and Fiji. A diffusion based passive sampling device comprising of microporous polyethylene (PE) for the long-term time-integrative monitoring of PFASs in aquatic environmental systems was used to monitor PFAS.

The objectives of this study were to characterise and identify the new types of PFAS that are present around the world using a non-target screening with QTOF-MS and to assess the sensitivity of PE passive sampling technique in sampling different types of PFAS.

Determination of perfluoralkyl substances in water by direct injection of matrix-modified centrifuge supernatant and LC/MS/MS

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Perfluoroalkyl substances (PFAS) are a growing concern with an EPA Drinking Water Health Advisory level of 70 ng/L for PFOS plus PFOA, and proposed guidelines as much as 10 times lower in other jurisdictions. The USGS National Water Quality Laboratory has developed LC/MS/MS methods for the determination of 34 of PFAS in surface water, groundwater, wastewater effluent, and other matrices. Target compounds include PFOS and PFOA, other sulfonates and carboxylates of varying chain length, and select precursors and synthetic substitutes (e.g., GenX, ADONA).

Sample preparation was streamlined with no filtration and minimal sample handling; field samples (1 mL) collected directly into centrifuge tubes were amended with isotopically-labeled standards and methanol (~50% by volume), centrifuged, and supernatant transferred to polypropylene vials for analysis. Compounds were separated on a porous shell reversed-phase column with a methanol-water gradient and analyzed by multiple-reaction monitoring in negative electrospray mode with isotope-dilution quantitation.

Method validation studies were conducted in groundwater, surface water, and wastewater effluent with replicates (n=7) spiked at multiple concentrations between 2 and 2000 ng/L. Recovery at intermediate concentration (145 ng/L) for 30 of 34 compounds ranged from 78.9 to 114.0% with RSDs less than 20.4%. Each matrix was spiked (413 ng/L), refrigerated, and recoveries estimated after t=0, 7, 28, and 90 days. Maximum holding time (28 days) was set as the longest time with all compound recoveries above 70%. Method detection levels (MDLs) determined in reagent water using a multi-concentration statistical approach (ASTM's DQCALC, 8 concentrations) ranged from 1.5 to 21.3 ng/L.

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Title: Tailoring stream restoration designs to optimize removal of stormwater contaminants

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Abstract (250 word limit): Urban stormwater often contains hundreds to thousands of individual pollutants. Land-based green infrastructure is a popular strategy to treat pollution, but fugitive stormwater can still reach the stream corridor by draining from lands with insufficient green infrastructure coverage. Indeed, more than half of all rivers and streams in the U.S. are degraded, and the fastest-growing cause of impairment is urban nonpoint source pollution. Stream restoration is a promising option to enhance the contaminant attenuation capacity of receiving waters, but practitioners lack clear design guidance to tailor restoration designs to specific contaminants of concern. In this study we address the design-to-function knowledge gap with paired field and numerical modeling of stream restoration structures on Thornton Creek, the largest and most urbanized watershed in Seattle, WA. Field monitoring showed that half of the ~1,200 detected organic contaminants were removed by >50% in the hyporheic zone (streambed sediments) beneath restoration structures. This included many emerging and unknown compounds, including a subset that were correlated with coho salmon pre-spawn mortality. Field data also showed that pollutant removal increased with hydraulic retention time through the hyporheic zone. Subsequent numerical modeling showed that the mean residence time and broader residence time distribution of hyporheic flowpaths can be increased by structural design decisions. Such design modifications would allow practitioners to optimize treatment to specific pollutants of concern and improve water quality in stormwater-impaired receiving waters.

Title: Transformation Product Formation Upon Heterogeneous Ozonation of the Tire Rubber Anti-Oxidant N-1,3-Dimethylbutyl-N-Phenyl-P-Phenylenediamine

Authors: Ximin Hu[1], Haoqi Zhao[1], Zhenyu Tian[2,3], Katherine Peter[4], Edward Kolodziej[1,2,3] and Michael Dodd[1]

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Abstract: Transformation products (TPs) are a class of widespread emerging contaminants whose environmental fate and risks are poorly understood. TPs originating from tire tread wear particles (TWP) can be generated throughout the tire rubber lifetime and may be transported to surface waters following storm events, in turn presenting a source of chemical exposure to aquatic life and humans. Our study investigated TP formation occurring during heterogeneous reaction of gas-phase ozone with the common tire rubber antioxidant 6PPD (N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine), both as a pure compound and as a constituent of TWP. Oxidative transformation of pure 6PPD was observed during exposure to ozone, with 81% of total 6PPD mass reacting during 6-hours of exposure on the 6PPD coated slide. Conversion molar yield of 6PPD to 6PPDQ – a recently reported highly toxic TP – was confirmed from the investigation. The TWP ozonation was conducted as the similar manner as pure compound. By aligning the potential TP features from ozonation, we thus prioritized 20 unique 6PPD-associated TPs that were found in both ozonated 6PPD and TWP samples, underscoring the importance of 6PPD as a primary antioxidant in tire rubber products and major TP source when tire rubber is subjected to ozone exposure. Additionally, by screening environmental samples, we prioritized 9 TPs that formed from 6PPD ozonation as also being prevalent in receiving waters impacted by roadway runoff. The data imply that tire rubber antioxidants react with ozone to form various TPs that are released throughout the tire rubber service life and have potential impacts on aquatic environments.

Influence of salinity on pyrethroid toxicity: behavior in a model estuarine organism (*Menidia beryllina*)

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Presentation type: Oral Presentation but I am also okay with a poster presentation if oral presentation slots are filled

Climate change is causing changes in precipitation patterns and contributing to increased sea levels. These alterations are linked with changes in salinity in estuaries, making the differences in toxicity across a salinity gradient a topic of increasing interest in assessing risk to estuarine fish species. Several recent studies have shown that pyrethroid toxicity can change across a salinity gradient. Pyrethroid pesticides are commonly used globally in agricultural, industrial, and household settings. Early life exposures in fish to pyrethroids has been found to cause toxicity at environmentally relevant concentrations and alter behavior, which has been demonstrated to be a sensitive endpoint that can detect toxicity of environmentally relevant concentrations of aquatic pollutants. Therefore, Inland Silversides (*Menidia beryllina*), a commonly used euryhaline, model fish species, were exposed from 5 days post fertilization (approximately 1-day pre-hatch) for 96 hours to six pyrethroids: bifenthrin, cyfluthrin, cyhalothrin, permethrin, cypermethrin, and esfenvalerate. Exposures were conducted at three salinities relevant to brackish, estuarine habitat (0.5, 2, and 6 PSU) and 3 concentrations, either 0.1, 1, 10, and/or 100 ng/L, determined from previous experiments to be sublethal and environmentally relevant. After exposure, Silversides underwent behavioral assays and were subjected to a dark and light cycle to determine behavioral toxicity. Results show significant behavioral changes with each pyrethroid exposure at all salinities and concentrations. These results indicate that there may be different behavioral responses to pyrethroids depending on pyrethroid type and salinity. These data will provide knowledge to managers and environmental planners to help further protect threatened and endangered fishes in estuarine and bay regions.

Comparing the limits of detection of different Fourier transform infrared spectroscopy techniques for the detection, quantification and identification of microplastics

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Abstract:

Microplastics are now widely acknowledged as a significant environmental pollutant, and can be found in soils, natural waters, biota and animals. Microplastics are typically considered to have a size range spanning five orders of magnitude, from the sub-micron to millimetre range. In order to fully understand the source, distribution, transport, fate and impact of microplastics in the environment it is necessary to be able to accurately physico-chemically characterise them. While the detection and characterisation of microplastics in the upper range of the size distribution is reasonably straight forward, as the size of the particles reduces, it becomes more challenging to characterise them appropriately. To do so accurately, it is essential to ensure that the testing instrumentation is fit-for-purpose for the sample under study and to understand the limitations of the technique being used for characterisation.

In this study, we aim to assess the limit of detection (LoD) of different Fourier-transform infrared (FTIR) spectroscopy techniques, including microscopy FTIR (µFTIR), attenuated total reflection (ATR-FTIR) and the hyphenated thermogravimetric analysis (TGA) – evolved gas analysis FTIR. For each technique suitable reference materials have been used as a challenge, including certified size standards of spherical polystyrene latex (PSL) particles, along with other well-defined polymer materials. The approach described here can also be modified for a range of other commonly used techniques such as Raman spectroscopy, scanning electron microscopy or other methods.

Ethylene oxide emissions and risk of breast cancer and Non-Hodgkin lymphoma in a large U.S. cohort

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Background: Ethylene oxide (EtO) is a carcinogenic gas used to sterilize medical equipment; emissions increased dramatically during the COVID-19 pandemic. We investigated the relationship between environmental EtO exposure and risk of two *a priori* suspect cancers based on limited occupational studies.

Methods: Using the U.S. Environmental Protection Agency's Toxics Release Inventory (TRI), we estimated historical exposures (1987-1995) for NIH-AARP Diet and Health Study participants enrolled in 1995-1996. Distance-weighted average emissions indices (AEI=∑[lbs EtO/km^2]) reflected the sum of annual emissions for all TRI facilities within 3,5, or 10km of the residence, also weighted by the proportion of time the home was downwind of the facilities. We evaluated incident Non-Hodgkin lymphoma (NHL; n=1,671 cases) in the full cohort (N=451,945) and breast cancer (n=3,796 invasive and *in situ*) among postmenopausal women (N=173,670), overall and by subtype and disease characteristics.

Results: We observed a non-significantly increased risk of breast cancer overall in the 95th AEI percentile within 3km (hazard ratio $(HR)_{[P95.vs.0]}$=1.48,CI=0.93-2.35). Risk of breast cancer *in situ* increased with the AEI within all distances evaluated; however, the strength of the associations declined at larger distances ($HRs_{[Q4.vs.0]}$=1.67,1.55,1.29 at 3, 5, and 10km respectively). No differences were observed by hormone receptor status. We found no clear pattern of elevated NHL risk overall, with non-monotonic and non-significant increases for CLL and follicular lymphoma subtypes.

Conclusions: A positive association between EtO emissions and risk of *in situ*, but not invasive, breast cancer warrants additional evaluation of this re-emerging exposure. Observed differences by stage may have mechanistic implications.

Potential for Bioelectrochemical Degradation of BPA

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More than one million pounds of Bisphenol A (BPA), a common monomer feedstock utilized to synthesize polycarbonates and epoxy resins, are discharged into the aquatic environment annually. Owing to its widespread use, its prevalence in the environment, and studies demonstrating estrogenic and genotoxic effects of this chemical on humans, BPA has been classified as a contaminant of emerging concern. Therefore, finding an efficient mechanism for removing BPA during water treatment is essential to protecting the environment and mitigating the risk to human health. This study analyzed the ability of *E. coli* and *S. oneidensis* to degrade BPA. Four microbial strains were incubated with shaking at 30 °C for 24 h in Luria-Bertani (LB) broth spiked with 1 μg/L of BPA. BPA was subsequently isolated using solid-phase extraction (SPE) and concentrated under N_2 evaporation. The BPA samples were quantified using liquid chromatography-tandem mass spectrometry (LC-MS/MS) employing selected reaction monitoring (SRM). Relative to the positive control (LB spiked with BPA), a 60% to 70% reduction in BPA was observed, indicating microbial degradation of this emerging contaminant of concern. This study provides baseline degradation levels for future bioelectrochemical degradation experiments of BPA.

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Alteration of the Neonicotinoid Insecticidal Pharmacophore Drives Differences in Parent and Product Sorption: Experimental, Field, and Modeling Results

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Recently, we reported the initial discovery of neonicotinoid insecticides and their metabolites in finished drinking water, and subsequent discovery of novel chlorinated neonic-derived disinfection byproducts. Neonicotinoids are part of a growing class of target-specific pesticides, wherein receptor binding propensity is conferred through a specific structural pharmacophore (e.g., an electronegative nitro-/cyano-group). Although neonicotinoids were not removed via conventional drinking water treatment, GAC was surprisingly effective for these high-solubility (i.e., low Kow) compounds, as demonstrated by analysis of long-term exposed spent GAC from a full scale DWTP. We hypothesized that the insecticidal pharmacophore impacted sorption to black carbon, and that removal of structurally altered neonicotinoid metabolites was inhibited. In this work, we demonstrated that neonicotinoid sorption to black carbon is extensive and largely irreversible. We characterized differences in sorption between neonicotinoid parent compounds and pharmacophore-altered products using functionalized (COOH- and NH_2-) and non-functionalized carbon nanotubes and GAC. Results indicate the electronegative pharmacophore drives sorption propensity, and presumed mechanisms likely differ between parents and products. The hypothesized mechanisms of neonicotinoid sorption extend beyond bulk hydrophobic interactions (i.e., electrostatic and hydrogen bonding), rendering currently available prediction models (e.g., pp-LFERs/LSERs) inadequate for neonicotinoids. The lack of commercially-available authentic standards for novel transformation products led us to develop a new QSAR-based model to predict neonicotinoid partitioning using QSAR descriptors that best reflect neonicotinoid interactions that drive partitioning between octanol-water and carbon-water systems. We were able to accurately model (and externally validate) neonicotinoid partitioning, and subsequently predict partitioning of novel neonicotinoid transformation products.

Spatial and Temporal Variability of Complex Pharmaceutical Mixtures and their Impacts in a Temperate-region Wastewater Effluent Dominated Stream

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An important pathway for contaminants of emerging concern in wastewater is pharmaceutical loading to the environment from incomplete removal in wastewater treatment plants (WWTPs). Wastewater effluent-dominated systems represent worst-case scenarios because pharmaceuticals are continuously discharged into a relatively small/less diluted water system. To understand the spatial and temporal dynamics of pharmaceuticals and their corresponding effects to aquatic organisms in temperate regions, a small effluent-dominated stream in Iowa was selected as a field laboratory for study. Four strategically located sampling sites were selected for this study: 1) above the WWTP outfall, 2) the WWTP outfall, 3) ~100 m below the WWTP outfall, and 4) ~5 km downstream. For a 12-month period, water samples were collected during low-flow conditions on roughly a biweekly basis and analyzed for 13 pharmaceutical compounds using a method by UIowa and collected monthly and analyzed for 110 pharmaceuticals using a method by the USGS. For monthly samples, the top 13 pharmaceuticals in terms of concentration accounted for over 85% of the overall chemical mass in a preliminary analysis. Spatial and temporal changes in total pharmaceutical loading, relative compound representation, and parent-to-product ratios demonstrate differential complex mixture attenuation that results in changing biotic exposure conditions. We calculated risk quotients for aquatic organisms under measured baseflow conditions and conducted stochastic risk modeling to estimate RQs under all-flows conditions. Ongoing efforts are relating pharmaceutical concentrations and total estrogenicity to in vitro zebra fish assays to better understand potential environmental impacts from exposure to pharmaceutical mixtures.

Title: Virus emissions from toilet flushing: comparing urine diverting to mix flush toilets

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Abstract

Shared toilets can be a source of exposure to pathogenic viruses. As many as 10^{10} - 10^{11} enteric viruses can be excreted per gram of feces during diarrhea.[1] When flushed, toilets generate virus-laden droplets that can remain viable in the air for up to 4 hours post flush (aerosols) or settle onto local surfaces (droplets).[2-4] The extent of virus emissions from toilet flushing depends on the toilet bowl volume, flush energy, and type.[5] This is an important consideration when designing and implementing different types of toilets.

One type of toilet that can have important implications for exposure to urinary tract and enteric viruses is urine diverting toilets. Physical separation of urine from the rest of the waste stream can remove a majority of the urinary tract viruses from the waste stream and mitigate emission during flushing. Consequently, it is important to distinguish between emission levels of urinary tract and enteric viruses and how the respective matrices impact emissions.

Ultimately, we performed a comparative assessment of urinary tract and enteric surrogate virus emissions from a urine diverting and a mix flush toilet and evaluated the impact of protein content in the matrix on virus emissions during a toilet flush. The results of this work demonstrate that infectious viruses can be emitted during toilet flushing and that virus emissions are impacted by the protein content of the matrix. It is important to consider user exposure to viruses when implementing different types of toilets and sanitation technologies. This work can bring focus to the gaps in understanding exposure to infectious viruses in shared toilet settings.

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Critical role of semiquinone in the reductive dehalogenation

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Abstract

Quinones (QNs) are ubiquitous and play a significant role in mediating electron transport in natural and biological systems. The redox reactivity of natural organic matter (NOM) and biochars (BCs) have been attributed to their quinone components, although there is a lack of direct evidence. In this study, we examined the reactions between triclosan (TCS) as a model organohalogen and hydrobenzoquinone (BHQ). We found that when TCS was mixed with BHQ in the molar ratio of 1:1 at pH 3, 5, and 7, no TCS degradation was observed under either oxic or anoxic conditions indicating that BHQ cannot reduce TCS within the experimental period. In the mixture of TCS, Fe(III), and BHQ, TCS was degraded substantially at pH 5 and 7 with half–life of around 57 and 18 hours under anoxic conditions. In the presence of O_2*, degradation of TCS was shut down completely. At pH 3, no degradation of TCS was observed in the presence and absence of* O_2*. The control experiment for the Fe(II) system mixed with TCS showed that no degradation of TCS was observed in the presence of Fe(II). The observed reaction between TCS and HQ in the presence of Fe (III) at pH above the pKa of BSQ (pKa = 4.1) suggests the importance of the deprotonated* BSQ^- *in their reaction with TCS. A kinetic model was built to predict the rate constants of the critical reactions.*

Title: Effects of Wear Processes on Per- and Polyfluoroalkyl Substances in Firefighter Turnout Gear Textiles

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Abstract: Firefighter serum concentrations of certain per- and polyfluoroalkyl substances (PFAS) have been observed to be elevated compared with the general population and to increase with years of service. One potential PFAS exposure pathway of special relevance to firefighters is contact with personal protective equipment (PPE) that is composed of or treated with fluoropolymers. To determine if contact with PPE could expose firefighters to PFAS, the concentrations of 55 PFAS were determined with LC-MS/MS and GC-MS in textiles used in the production of firefighter turnout gear. Up to 30 PFAS were quantified in individual textiles, at concentrations up to 350 ng/g. Additionally, the effects of wear processes, including exposure to ultraviolet radiation, laundering, abrasion, and heat were evaluated to determine how typical use may alter PFAS composition in firefighter gear. Laundering and exposure to heat lowered the overall concentration of extractable PFAS in the turnout gear textiles, while abrasion increased extractable PFAS concentrations. Measured concentrations of shorter chain perfluorocarboxylic acids decreased with UV irradiation, while those of longer chain homologs increased. The presence of PFAS in turnout gear textiles as well as the changes in concentration following exposure to wear processes indicates that firefighters may be exposed to PFAS from both new and in-service turnout gear.

Microbial biotransformation of dichloroacetamide herbicide safeners in river sediment microcosms

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Herbicide safeners are a class of biologically-active agrochemicals commonly included in commercial chloroacetamide herbicide formulations to selectively protect crops against herbicide toxicity. Dichloroacetamide safeners are hydrophilic ($\log K_{ow}$ 1.84 – 3.19) and mobile in aqueous environments, which has led to their detection in Midwestern drinking water sources at concentrations up to 190 ng/L. Although safeners demonstrate toxicity toward non-target organisms, they are classified and regulated as “inert” constituents under the U.S. Federal Insecticide, Fungicide, and Rodenticide Act and similar international legislation. Recent studies suggest that dichloroacetamides can transform over environmentally-relevant timescales into products with increased bioactivity that may pose human and environmental health risks. However, the fate and effects of dichloroacetamides and their transformation products remain largely uncharacterized. To evaluate dichloroacetamide fate, we quantified relative timescales, elucidated transformation pathways, and identified novel products of microbially-mediated safener transformation in aerobic microcosms containing river sediment. The safener benoxacor, unlike its herbicide co-formulant metolachlor, undergoes a multistep, co-metabolic microbial transformation reaction through a monochlorinated intermediate to yield a glutathione conjugate. This is notable as prior investigations have demonstrated toxicity of the monochloro-benoxacor intermediate toward insect larvae. Ongoing studies are assessing the microbial transformation of another dichloroacetamide safener, dichlormid; transformation of dichlormid via the same microbial pathway as benoxacor would result in the formation of the active herbicide CDAA. These studies help expand our understanding of safener fate in aquatic environments building upon our prior work on their photolysis, hydrolysis, and reductive dechlorination.

TITLE: *In vitro* predictions vs. *in vivo* reality: Molecular impacts of exposure to WWTP effluent in zebrafish embryos are partially predicted from aggregated ToxCast data

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ABSTRACT:

Wastewater treatment plant (WWTP) effluent-dominated streams provide critical habitat for aquatic organisms but also continually expose them to complex mixtures of pharmaceuticals that can potentially impair growth, behavior, and reproduction. Limited data on the adverse biological impacts of these exposures make it difficult to assess exposure risks, particularly with respect to pharmaceuticals whose designed bioactivity often extends beyond conventionally monitored biological pathways. Thus, the aggregation of known biological impacts from *in vitro* high-throughput assays in the ToxCast database provides critical insight for chemical mixture prioritization and assessment of biological risk. This study compares the conclusions of cumulative risk screening using ToxCast data to targeted and global gene expression of *Danio rerio* (zebrafish) embryos exposed to water samples from a WWTP effluent-dominated stream. These environmental samples were concurrently evaluated for 113 pharmaceuticals and other contaminants of emerging concern. This work identifies biological processes and pathways responsive to *in vivo* effluent exposures that are missing from ToxCast database. Zebrafish embryos at two developmental stages were exposed to monthly water samples collected at baseflow conditions from four sampling sites (100 m upstream, at the effluent outfall, 100 m below the outfall, and 5 km below the outfall) between January and August 2018. ToxCast risk screening generated potential molecular effects that were also identified in gene expression data from *in vivo* zebrafish embryo exposures, including effects related to cardiac and muscle development. However, other effects identified through the *in vivo* exposures were not captured by ToxCast assays and included metabolic and visual system impacts. This work demonstrates a need to expand coverage of biological processes within the ToxCast database to encompass molecular effects specific to pharmaceutical mixtures in WWTP effluent.

Occurrence and distribution of pharmaceuticals in surface water and sediment of Buffalo and Sundays River estuaries, South Africa and their ecological risk assessment

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ABSTRACT

This study investigated the presence of pharmaceuticals in the water and sediment of Buffalo and Sundays River Estuary, South Africa. Extraction for water and sediment samples was achieved with solid-phase extraction and ultrasonic extraction methods, respectively. Quantification of the target analytes was done with UPLC-QTOF-MS. The pH of surface water in all the sampling sites (8.18-10.1) were above the WHO guideline (6.0 to ≤ 9.0). A good correlation was observed between the analytes and organic matter and organic carbon. Results showed that carbamazepine exhibited the highest concentration (8.75±1.45 µg/kg) of all the pharmaceuticals, while trimethoprim has the highest detection frequency with the highest concentration of 1.62 ± 0.83

µg/kg in the sediment samples. Sulfamethoxazole was below the detection limit in both estuaries. Calculated risk quotients revealed that carbamazepine and trimethoprim could be of potential risk, while caffeine may pose a very low risk to the aquatic organisms investigated. Proper monitoring of the runoff entering Buffalo Estuary is required, being the point of discharge of Buffalo River to the Indian Ocean. Also, the domestic waste discharge from residences in the surroundings of Sundays Estuary should be monitored.

Title: Synthesis of ferrate-coated sand and application for urban stormwater treatment

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Abstract:

Recent studies highlighting the toxicity of organic pollutants in urban stormwater indicate the need for an effective treatment media such as ferrate (Fe(VI)) capable of simultaneous oxidation of organic compounds and adsorption of heavy metals in water. The reduction leads to the formation of in situ non-toxic Fe(III) oxide phases, making Fe(VI) an environmentally friendly technology for water treatment. However, in aqueous solution, Fe(VI) can decay rapidly into Fe(III) which impedes Fe(VI) reactivity toward organic contaminants. Previous studies showed that silica (SiO_2), the main component of sand, can increase the oxidative capacity of Fe(VI) by retarding its self-decomposition. Here, we leveraged the property of SiO_2 Fe(VI) stabilization to develop a Fe(VI)-coated sand media for urban stormwater treatment infiltration applications. The sand is first mixed with a tetraethyl orthosilicate for activation which acts as a Fe(VI) binding agent. The degradation and complexation capacities of the Fe(VI)-coated sand was evaluated using pentachlorophenol and copper as representative urban stormwater contaminants. Physical and chemical properties (i.e., oxidation state and chemical binding of Fe) of the Fe(VI)-coated sand were characterized by surface analyses and colorimetric methods were used to determine the rate and speciation of Fe leached from the media surface. Our results show that the ferrate-coated sand can treat pentachlorophenol and copper in aqueous solutions to levels safe for urban stormwater discharge. The results of this study demonstrate the potential application for Fe(VI)-coated sand in the treatment of multiple types of pollutants in urban stormwater infiltration systems.

Assessing Reliability of Non-Targeted High-Resolution Mass Spectrometry Fingerprints for Quantitative Source Apportionment in Complex Matrices

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Differentiating and deconvoluting contaminant source impacts in complex environmental systems is key to effective management. Existing approaches that rely on targeted chemical analyses are limited when pre-selected analytes occur below detection limits and/or are derived from multiple contaminant sources. Non-targeted analyses that leverage high-resolution mass spectrometry (HRMS) yield rich datasets that characterize much sample-specific chemical composition, providing additional potential end-members for source differentiation and apportionment. Previous work demonstrated that HRMS source fingerprints can define sample uniqueness and support accurate, quantitative source concentration estimates. Here, using two aqueous film-forming foams as representative complex sources, we assessed the qualitative fidelity and quantitative accuracy of HRMS source fingerprints in increasingly complex background matrices. Across all matrices, HRMS-derived source apportionment estimates were 0.9 ± 0.12-fold and 0.73 ± 0.26-fold of actual in samples impacted solely by analytical matrix effects or by sample processing recovery and analytical matrix effects, respectively. Isotope-labeled internal standards could not be readily paired to individual unidentified non-target features, but bulk internal standard-based feature abundance corrections improved apportionment accuracy in higher matrix samples (from 0.79 ± 0.1-fold to 0.96 ± 0.1-fold of actual) and/or informed source concentration estimate relative error. Data mining to identify individual chemical end-members within HRMS fingerprints yielded 16 PFAS and hydrocarbon surfactant homologous series. Although additional studies are needed to assess the analytical repeatability, transferability, and environmental persistence of HRMS source fingerprints, the results further demonstrate the potential application of non-targeted HRMS data for source apportionment and other quantitative outcomes.

Hydrothermal Processing for Emerging Contaminant Treatment

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The widespread use of per- and polyfluoroalkyl substances (PFAS) in aqueous film forming foam (AFFF), manufacturing processes, and consumer goods has caused widespread contamination of groundwater and soil, both in the US and abroad. Military bases, commercial airports, hydrocarbon storage facilities, and firefighter training centers are all hotspots for "forever chemical" contamination, which must be actively remediated, due to the high toxicity and bioaccumulative potential of PFAS. While several technologies are effective in separating PFAS from contaminated water or soils, end-of-life destruction of remediation byproducts and PFAS-rich substances remains a pressing challenge.

Hydrothermal processing shows great promise as an emerging PFAS destruction technology, with low energy requirements and complete effectiveness over the entire family of PFAS compounds. In this talk, Aquagga's hydrothermal PFAS destruction technology, currently under development in partnership with the University of Washington, will be introduced. Additionally, the results of several recent case studies conducted with bench-scale systems will be presented. These include studies in both batch and continuous reactor configurations, demonstrating the ability to safely destroy >99.999% of PFAS in contaminated liquids such as raw AFFF and contaminated groundwater samples. Current efforts towards scale-up and pilot system deployment will also be presented.

Title: Catalytic, reductive defluorination of per- and polyfluoroalkyl substances by vanadium carbide MXenes and hydrogen peroxide

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Abstract (oral preferred): Per- and polyfluoroalkyl substances (PFAS) are synthetic organic chemicals with high thermal stability which lends itself to use in many consumer-end products. Production and use of these chemicals has contributed to their widespread dispersion in environmental waters, and exposure to PFASs have been linked to negative toxicological and epidemiological health effects in humans and mammals. Advanced reduction processes in which solvated electrons are generated has emerged as a promising approach to degrade PFAS in water. Reductive defluorination of PFAS in water requires alkaline pH and anoxic conditions to prevent scavenging of solvated electrons. To maximize defluorination, it is beneficial to co-located solvated electrons and adsorbed PFAS on substrate surfaces; however, there are limited substrates available capable of generating solvated electrons without continuous energy inputs (e.g., ultraviolet light) and/or chemical mediators (e.g., sulfite). In this study, we employ vanadium carbide (V_2C) MXenes—a new family of two-dimensional, early transition metal nanomaterials—to serve as a reactive substrate for treatment of perfluorooctane sulfonate (PFOS), a representative PFAS. Addition of hydrogen peroxide (H_2O_2) catalyzed the two-electron reduction of vanadium(V) phases within the V_2C to vanadium(III) which led to formation of solvated electrons near the V_2C nanosheet surface where PFOS was adsorbed. 50 µg/L PFOS decreased by 96% within 4 h in the presence of 0.15 mg/mL V_2C nanosheets and 14.7 mM H_2O_2 in ultrapure water under aerobic conditions which corresponded to near-complete defluorination. This unique and effective reaction system could be leveraged to treat other persistent compounds in water.

Combining passive sampling sorbents and Non-Target Analysis (NTA) for comprehensive characterisation of contaminants of concern in environmental water systems

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Modern water pollution is complicated by diverse contaminants, their intermittent release and environmental transformation. Traditional sampling and screening strategies for contaminants are restricted by their top-down approach focussing on a few regulated compounds. By reversing this paradigm and determining the actual chemical contaminant composition in our waterways we may be able to more accurately identify and evaluate the pollutants in our environment that may adversely affect environmental health.

A combination of techniques such as passive sampling, together with comprehensive high resolution mass spectrometry (HRMS) for analysis could provide a broader picture of the pollution.

Passive sampling can potentially provide in-situ extraction and concentration of samples in a time-integrative manner. Non-target analysis has the potential of identifying a wide range of features, beyond the limited set of target compounds, to help identify additional unknown or unexpected compounds in these samples. However, the validation of NTA methods and workflows with passive sampling extracts, that may contain problematic interfering features, has not been sufficiently studied.

For this study, we compare the performance and matrix constituents of 11 passive sampler sorbents (EVOLUTE WAX, EVOLUTE AX, EVOLUTE ABN, Sepra SAX, Sepra-ZT-WCX, Sepra-ZT, Sepra-ZT-WAX, ISOLUTE 101, ISOLUTE ENV+, DEXSORB+ & Coconut charcoal) when exposed to wastewater influent for 24 hours. After extraction, samples were analysed with liquid chromatography coupled to HRMS, providing insights into the differences between the sorbents and their matrix effects.

This comparison aims to determine how sampling techniques may influence results to develop a workflow for better characterisation of contaminants in water samples.

Abstract Title:

Quantifying Untargeted Metabolomic Changes in Watersheds and the Contribution of Putative Environmental Drivers

Authors:

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Abstract:

Dissolved organic matter (DOM) plays a significant role in watershed ecosystem metabolism and nutrients cycling, with further impacts on water quality and food security. However, the assemblages of tens of thousands of unknown and continuously changing organic molecules in an ecosystem, sometimes referred to as a metabolome, make it challenging to characterize the composition and determine the drivers of variation. The dynamic nature of untargeted metabolome records the information of upstream land-use sources and in-stream watershed processes. By screening a single water sample from the outflow of a watershed, it is theoretically possible to simultaneously quantify all ecosystem processes occurring upstream in a watershed simply by testing for the presence of the diagnostic metabolomic signatures (fingerprints). Therefore, it is critical to identify metabolomic signatures that are indicative of their sources and/or ecosystem processes. Advances in high resolution mass spectrometry (HRMS) and machine learning tools make it possible to decode watershed metabolomes. Our aim is to build upon these strategies to identify the different metabolomic signatures that are indicative of different land-use sources and watershed processes. In this study, we quantified the temporal and spatial variability of environmental metabolomes from 4 watersheds in northwestern Oregon. The preliminary results indicate strong seasonal variability in metabolomic composition. The findings suggest that seasonal ecosystem processes are the leading driver of the metabolomic changes, rather than spatial variation or land-use sources in these four watersheds. Metabolomic signatures of different land-use sources are also identified in each season. Future studies will develop fingerprinting workflow from watershed metabolomes with more diverse land-use sources and ecosystem processes.

Physicochemical and Organic Matter Partitioning Properties of Novel Brominated Flame-Retardants

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The compounds 1,2-bis-2,4,6-tribromophenoxyethane (BTBPE), decabromodiphenyl ethane (DBDPE), and pentabromobenzene (PBB) are among a group of “novel” flame retardants that have replaced polybrominated diphenyl ethers (PBDEs). To date the physicochemical properties of these compounds have been estimated based upon their structures using various linear free energy relationships (LFER) that have yet to be corroborated by experimental data. For this study we measured the aqueous solubility, n-octanol-water (K_{ow}), and dissolved organic matter partition coefficients (K_{DOM}) for these three novel flame retardants. Measurements were conducted using batch equilibrium approaches and compared to values estimated using both single parameter and poly parameter LFERs. DOM used in the study include both a reference material (Suwannee River Natural Organic Matter) and organic matter isolated from diverse watersheds.

Title: Chloride enhances viral genome reaction rates at conditions relevant to water treatment.

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Abstract:

The emergence of novel viruses, including SARS-CoV-2, and prevalence of difficult-to-culture and non-culturable viruses in the environment has increased interest in developing predictive models for viral inactivation during disinfection. To develop these models, a mechanistic understanding of how disinfectants inactivate viruses, and which disinfectant species drive inactivation, is desirable. Chlorination is used widely to inactivate viruses in water, and chlorine inactivates viruses by oxidizing viral components, including nucleic acids. To date, molecular biologists have assumed that hypochlorous acid/hypochlorite HOCl/OCl- is the chlorinating agent that initiates nucleic acid damage, and chlorination rates determined for viral genomes are grounded in that assumption. However, recent studies have underscored that minor constituents of chlorine, molecular chlorine (Cl_2), and dichlorine monoxide (Cl_2O), which exist in equilibrium with HOCl/OCl-, can influence chlorination rates of organic compounds, especially at elevated chloride concentrations (> 3 mM) in which they are favored to form. Here, we show that the first-order chlorination rates of dsDNA and ssDNA extracted from representative bacteriophages are enhanced in the presence of chloride. To our knowledge, this is the first study to show that chlorination rates of biological macromolecules are affected by chloride concentrations present at levels relevant to water disinfection. We further show that these enhanced chlorination reaction rates can be explained by the presence of Cl_2 and Cl_2O in solution. The results of this study will inform kinetic models for viral genome chlorination, and bring us one step closer toward accurate viral inactivation predictive models.

Proposed Process for Thermal Destruction of PFOA and PFOS by Municipal Solid Waste Derived Biochar

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Abstract

Per- and polyfluoroalklyl substances (PFAS) are an emerging contaminant that threaten human health and are difficult to destroy in the environment. Sustainable PFAS destruction technologies are needed to mitigate the spread of these emerging contaminants through groundwater systems. Many technologies are in development, but often lack industrial scale-up potential through limited economic viability. This study presents a sustainable theoretical process and design plan for a PFAS destruction facility. The facility destroys the most well-studied forms of PFAS, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS), given a polluted groundwater flow rate of 700 gpm containing combined PFOA and PFOS at 100 ppt. The design includes the creation of biochar from the organic fraction of municipal solid waste, the adsorption of PFAS onto this biochar, the thermal destruction of PFAS on the biochar with the addition of calcium hydroxide, and subsequent air pollution and technologies. The process is theoretically able to destroy PFOA and PFOS to less than 40 ppt at a cost competitive $0.09 per gallon. This design is explored through design calculations, life-cycle costing, life-cycle assessment, health and safety regulatory analysis, and a proposed public involvement plan. This analysis showcases how the system is scientifically capable of scale-up, economically viable, and promotes diversion of waste products for environmental remediation. Future research should be performed from this foundation to further improve the system's efficacy, viability, and sustainability.

The Environmental Fate and Effects of Antibiotic Resistance Genes and Small Interference RNAs From Genetically Modified Crops

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Increasing rates of global population growth have amplified food scarcity across the globe and ushered in the development of genetically modified (GM) crops. Modern crops that use small interference RNA (siRNA) and antibiotic resistance genes (ARGs) have become increasingly common in the United States. GM crops remain controversial due to the uncertainty regarding possible unintended effects on the environment. ARGs or siRNAs from GM crops may be released during plant decomposition and adsorbed by soil, which can persist across large time scales and can lead to possible uptake by soil microbial communities. These genes can potentially contribute to antibiotic resistance as well as disrupt nutrient cycling and soil fertility. Therefore, siRNAs and ARGs which are emerging contaminants are a problem. Further information on the environmental effects of these genetic constructs is required as well as research focused on the genetic transfer to belowground microbes, transport, and fate. **Thus, the goal of this research is to assess the fate of GM crop ARG and siRNA transgenes in soil and determine the ecological impacts of their transfer to microbes using laboratory-based experiments.** It is hypothesized that transgenes are persistent and motile in soils, and horizontal gene transfer can occur if the conditions are optimal for bacterial uptake. Comparisons of transgenes sequences have been performed and database research has been performed. Results suggest homology between transgenes and soil bacteria genetic sequences. The information has also been used to design soil reactors to determine the persistence and behavior of transgenes.

Title: Investigating Sea Otter Exposure to Microplastics Using Spraint and Diet Analysis

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Abstract: Sea otters act as valuable indicators of ecosystem health and consume prey items that contain microplastics. Microplastic ingestion has been shown to have a wide range of deleterious effects depending on the organism and plastic type. We are investigating the ingestion of microplastics by sea otters (*Enhydra lutris*) in Alaska and housed at the Seattle Aquarium by assessing the presence and abundance of microplastics in scat samples. We are also analyzing diet items of captive otters for microplastic particles to evaluate the role trophic transfer has in microplastic exposure for these individuals. Sample processing includes digestion of organic material with potassium hydroxide, a density separation using a hypersaline solution, and confirmation of potential plastics with FTIR spectroscopy. Preliminary results suggest that the majority of plastics in wild sea otter scats consist of fibers and fragments, in the colors blue, black, and clear. This study will provide information on the current level and type of microplastic exposure to populations of captive and wild sea otters using a non-invasive method, which may be beneficial for understanding sea otter population health.

RNA hydrolysis at mineral-water interfaces

(Proposal for an oral presentation)

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Double-stranded RNA (dsRNA) has been developed as a new type of pesticide in agriculture. Because the release of dsRNA pesticides to agricultural soils may pose potential ecological risks to nontarget organisms depending on dsRNA environmental concentrations, we need to understand dsRNA fate in soils. Like DNA, dsRNA fate in soils is expected to be determined by adsorption to particles or degradation degraded by nucleases. However, whereas DNA adsorbed to soil particles is widely reported to be protected from enzymatic hydrolysis and thus persist for extended time periods, we previously found that dsRNA adsorbed to soil particles degrades rapidly. To explain this difference, we hypothesized adsorption of dsRNA to metal (hydr)oxide minerals might catalyze phosphodiester bond hydrolysis. We determined dsRNA adsorbed to the mineral goethite underwent abiotic phosphodiester bond hydrolysis and validated this as the dominant mechanism by identifying monophosphate nucleotides as the primary reaction products. From these results, we proposed that mechanism of goethite-mediated RNA hydrolysis involves nucleophilic attack on phosphorus atoms facilitated by iron coordination. Other metal (hydr)oxides (e.g., aluminum oxide) could also catalyze RNA hydrolysis after hours of adsorption, indicating the reaction might be common in soils. We found solution constituents, like organic matter and orthophosphate, impeded the degradation by competing for adsorption sites with RNA. Finally, we validated the catalyzed hydrolysis was unique to RNA and didn't occur for DNA (e.g., by goethite). Our results suggest mineral-mediated RNA hydrolysis, a novel pathway, may explain why adsorbed dsRNA in soils does not persist like adsorbed DNA.

Biotransformation of Current-Use Progestins Dienogest and Drospirenone in Laboratory-Scale Activated Sludge Systems

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Abstract

Dienogest (DIE) and drospirenone (DRO) are two fourth-generation synthetic progestins widely used as oral contraceptives. Despite their increasing detection in wastewaters and surface waters, their fate during biological wastewater treatment is unclear. We investigated DIE and DRO biotransformation with representative activated sludge batch incubations and identified the transformation products (TPs) with high resolution mass spectrometry. DIE exhibited slow biotransformation (16-30 hr half-life) and went through a quantitative aromatic dehydrogenation to TP 309 (molar yields ~55%), an aromatic TP ~30% estrogenic as 17β-estradiol. DRO experienced more rapid biotransformation (<0.5 hr half-life), and 1,2-dehydrogenation formed the major TP 364 (molar yields ~40%), an anti-mineralocorticoid steroid named spirorenone. Lactone ring hydrolysis was another important biotransformation pathway for DRO (molar yields ~20%) and generated a pharmacologically inactive TP 384. Other minor biotransformation pathways for DIE and DRO included hydroxylation, methoxylation, and 3-keto and C4(5) double bond hydrogenation, and distinct bioactivities are also plausible for these TPs, including anti-gestagenic activity, antigonadotropic activity, and pregnancy inhibition effects. Thus, biotransformation of DIE and DRO during wastewater treatment should be considered in environmental hazard assessments of synthetic progestins, especially certain TPs including the estrogenic TP 309 of DIE and the anti-mineralocorticoid spirorenone (TP 364) of DRO.

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Direct injection analysis of oxypurinol and metformin in wastewater using hydrophilic interaction liquid chromatography coupled to tandem mass spectrometry

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The prevalence of gout and diabetes is increasing around the world accompanied with an increase in the use of related prescribed medications, allopurinol and metformin, respectively. High volume use of these two pharmaceuticals leads to the ubiquitous presence of their metabolites, oxypurinol and metformin, in the aquatic environment, especially in wastewater. However, there are limited analytical methods available for measuring these two metabolites in wastewater due to their high hydrophilicity. In addition, current sample pre-treatments including solid-phase extraction and freeze-drying are time and labour intensive. This study aims to develop and validate a sensitive and simple method using direct-injection LC-MS/MS for the simultaneous measurement of oxypurinol and metformin in wastewater. Seven different HPLC columns were tested for retention and separation of the compounds and a hydrophilic interaction liquid chromatography (HILIC) column was selected for further optimisation and validation. The optimised sample pre-treatment only required filtration through regenerated cellulose filter following dilution of filtrated wastewater samples with LCMS grade acetonitrile (wastewater: acetonitrile, 10:90, v/v). The new method was applied to 42 daily wastewater influents samples and 6 effluent samples collected from six Australian wastewater treatment plants. Both compounds were detected in all wastewater samples, ranging from 29.3-214.5 µg/L in influents and 2.2-53.3 µg/L in effluents for metformin, 24.6-248.2 µg/L in influents and 3.5-80.8 µg/L in effluents for oxypurinol. Our results demonstrated that a rapid and sensitive LC-MS/MS method is feasible for simultaneous assessment of diabetes and gout biomarkers using wastewater analysis.

Direct Analysis of Trace Contaminant-Microplastic Sorption Phenomena with Membrane Introduction Mass Spectrometry

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Abstract

The concerning impacts of microplastics on the aquatic environment have been widely recognized. In addition to direct physical and physiological effects on organisms, microplastics can influence the fate and distribution of trace organic chemical contaminants through sorption (adsorption and absorption) processes. We present the use of a direct sampling mass spectrometry technique to simultaneously follow the time-resolved, solution-phase concentration of contaminants at low parts-per-billion concentrations. A capillary hollow fibre polymer membrane probe is directly immersed in a complex sample solution containing both chemical contaminants and suspended microplastics. To directly monitor analyte concentrations in real-time as sorption occurs, a solvent acceptor phase flows through the probe, sampling the solution, and is then directly injected into an ion source of a mass spectrometer. We report both the short-term sorption kinetics and long-term equilibria phenomena of four contaminants (naphthalene, anthracene, pyrene, and nonylphenol) on four different plastics (low density polyethylene, high density polyethylene, polypropylene, and polystyrene). The initial sorption rates and the extent of sorption were normalized for surface area and found to be highly dependent on the type of plastic. Sorption of polycyclic aromatic hydrocarbon analytes were not appreciably affected by photochemical weathering of polyethylene, but the rate and extent of nonylphenol sorption was observed to increase markedly. This work can be extended to examine a broader range of contaminant/plastic combinations to further probe the intrinsic properties that influence sorption processes, ultimately improving our understanding of the behaviour of microplastics in the environment.

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