



INEF 2018

Annual Conference of the International Network of
Environmental Forensics



University of Utah, Salt Lake City, Utah, USA
June 25-27, 2018

www.rsc.org/inef



INEF 2018

Welcome to the International Network of Environmental Forensics (INEF) 2018 conference. INEF was founded in 2008 for the purpose of providing a forum for scientists, environmental consultants, regulators and attorneys to share the latest information, methods and findings regarding the use of environmental forensics. The conference will consist of plenary presentations, and oral and poster technical sessions.

In my view, environmental forensics has always been a point of intersection for multiple scientific disciplines. I first became aware of the term in the late 1990s, and at that time, it implied primarily chemical fingerprinting, oil spill forensics, and environmental science in support of litigation. Twenty years on, if you scan this year's program, you will find those disciplines still well-represented, but there are also presentations on topics that go beyond those mainstays, including multidimensional chromatography, sophisticated data analysis/visualization methods, and novel ways of evaluating fate and transport of contaminants. We have a very strong program this year with over 75 presentations on a wide variety of environmental topics. We also have an outstanding group of plenary speakers that we hope will inspire INEF delegates to consider the possibilities and future directions of environmental forensics.

After the conclusion of INEF 2017 in Beijing last summer, INEF 2018 belonged to the INEF Committee (Gwen O'Sullivan, David Megson, Steve Mudge and Mike Fowler). A few months ago, it started to become mine. But now, INEF 2018 is yours. We hope these three days provide you with a cordial, informal opportunity to share ideas, and learn about the work of your fellow delegates. The organizing committee thanks the sponsors for generously supporting this event as well as all of the speakers, presenters and student volunteers for contributing their time and effort to make this a successful conference.

Kind Regards,



Glenn Johnson
INEF 2018 Chair
University of Utah, Salt Lake City, Utah, USA

INEF Committee

Gwen O'Sullivan	Mount Royal University, Calgary, Alberta, Canada
David Megson	Manchester Metropolitan University, Manchester, England, UK
Steve Mudge	Norwegian Institute for Air Research (NILU)
Mike Fowler	University of Portsmouth, Portsmouth, England, UK

Conference Organizing Committee

Ben Williams	University of the West of England, Bristol, England, UK
Sri Chaudhuri	Conservation Ontario, Toronto, Ontario, Canada
Eric Reiner	Ontario Ministry of the Environment and Climate Change, Toronto, Ontario, Canada
Paul Philp	University of Oklahoma, Norman, Oklahoma, USA
Emily Vavricka	EEC Environmental, Orange, California, USA
Michael Wade	Wade Research, Inc. Marshfield, Mass., USA.

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GENERAL INFORMATION

Venue

The conference venue for INEF 2018 is the **Fort Douglas Officers Club** at the University of Utah. This building dates back to 1875, when Fort Douglas was a small U.S. Army post. This will be the location for all plenary presentations, oral breakout sessions and posters (Layout on page 44).



Fort Douglas Officers Club

Lunches and dinners will be served at the **Heritage Center**, located a 5-10 minute walk, east of the Officer's Club (Map on p. 44). For INEF delegates staying at conference hotel (University Guest House) breakfast is included with your room.

The official hotel for INEF 2018 is the **University Guest House**, located next door to the Officers Club.

INEF 2018 social events include a Waters Welcome Reception at the **Natural History Museum of Utah**, and a Saints and Sinners night, with an Ice Cream Social at the Officers Club, and an optional downtown Salt Lake City Pub Crawl.

Registration Desk

Registration will be in the East Foyer. Early registration is available on Sunday, June 24 between 1:00pm and 5:00pm at the Officer's Club. On Monday, June 25, registration will open at 8:00am, approximately ½ hour before the Welcome and Introduction at 8:30am. The INEF 2018 registration desk will be open during the following hours:

Sunday (Officers Club, East Foyer)13:00 to 17:00
Monday (Officers Club, East Foyer)08:00 to 17:00
Tuesday (Officers Club, East Foyer)08:00 to 12:00
Wednesday (Officers Club, East Foyer).....08:00 to 12:00

Presenter Information

Each day there will be a short introduction/orientation at 8:30 or 8:45, followed by plenary talks at 9:00am, and concurrent technical sessions and posters through the remainder of the day. A detailed schedule is provided on pages 7-9.

Oral Sessions. Presenters in oral sessions are asked to provide their presentations in Microsoft PowerPoint format, on disc or flash drive, to the student volunteer or chair of your session, at least 30 minutes prior to the beginning of their session. Presentation should be approximately 15 minutes with 5 minutes for questions. Each speaker will be provided with a laptop, projector and microphone for their presentation.

Poster Sessions. We will have printed (hardcopy) posters in the poster sessions this year. The poster mounting boards will be available by 8:00 am Monday June 25, in the East Conference Room. Poster presenters are asked to hang their posters on Monday between 8:00am and the first coffee break after the plenaries (10:30am). Poster presenters' names will be indicated on the mounting board, where their poster should be displayed. Material for hanging posters will be made available at each poster stand. Recommended poster dimensions will be 36 inches wide x 42 inches tall (92 cm x 107 cm). Posters will be displayed on through 5:00 pm on Tuesday June 26. Authors of posters should be available to discuss content during the afternoon coffee/refreshment breaks on Monday and Tuesday (see schedule).

Publication of Proceedings

Contributions made by researchers at the conference will be made available in two formats; the collection of abstracts in this program (which is also available in electronic format on the INEF 2018 website) and as a published proceedings. Abstracts are arranged according to the individual day, time period and session according to program schedule.

Each year presenters are encouraged to submit manuscripts based on the contents of their presentations. These manuscripts are assembled and published as an open-access peer-reviewed collection. If your manuscript is accepted for publication INEF will cover your publication costs. We have a deadline of September 15 for all submissions. Manuscripts submitted after this date will not be considered.

A MS Word template and details of how to prepare an abstract and can be found on the INEF 2018 conference website (<http://www.rsc-inef.net/publications.html>), or by emailing editors of the proceedings issue Dr. David Megson (D.Megson@mmu.ac.uk) or Dr. Gwen O'Sullivan (gosullivan@mtroyal.ca). Your manuscript will then be reviewed by at least two reviewers and returned to you. If you are interested in helping with the peer review process, or have any other questions about the publication process, please contact either David or Gwen.

Access to Wireless Network

The **UGuest** wireless network will work at both the Officers Club and the University Guest House. Instructions to connect are:

1. Select the wireless network **UGuest** from the list of available wireless connections.
2. Open your Internet browser and go to *onboard.utah.edu*.
3. Agree to the Terms and Conditions and then click *Start*.
4. Follow the instructions on your screen.

If you require assistance, please contact the Campus Help Desk at 801-581-4000 or by dialing 1-4000 from your room phone at the Guest House (Select option 1). If you are still having trouble, contact the Guest House Front Desk (801-587-1015) and they will be happy to assist you.

Keep in Contact

The International Network of Environmental Forensics (INEF) is a non-profit, interest group within the Royal Society of Chemistry (RSC). It was founded in 2008 to provide a forum for scientists, environmental consultants, regulators and lawyers to share information regarding the use of environmental forensics. Environmental forensics is the use of scientific techniques to identify the source, age and timing of a contaminant into the environment. Join us at

<http://www.rsc.org/Membership/Networking/InterestGroups/INEF/>

INEF is involved with the design and delivery of a number of outreach programs, including conferences and workshops, to interested parties throughout the world. Information shared through these outreach programs provide investigators employing environmental forensic techniques with the most current scientific information available to identify the source, age and timing of contaminant release to the environment. You can keep up with INEF on social media via Facebook, Twitter (@INEF_net), and through our website. We invite you to share your experiences of the conference.

You will get a couple of emails from us over the next few months related to conference follow-up matters, such as instructions for manuscript submittal for the conference proceedings volume. It is our data protection policy to not distribute personal data (names, email addresses, etc.) to third parties without your permission. Your name and email address will be stored electronically by the INEF committee and we may use this data occasionally to inform you about

future INEF events. You have the right to opt out by contacting David Megson (d.megson@mmu.ac.uk).

Student Paper Competition

INEF has an active student outreach program with the express purpose of encouraging students to pursue studies in environmental forensics. A committee will review submitted student oral and poster presentations during the conference. The committee will select the four best student presentations and present them with cash rewards, as follows.

- 1st Prize:** \$750 (Sponsored by Infometrix)
- 2nd Prize:** \$500 (Sponsored by Daniel B. Stephens & Associates)
- 3rd Prize:** \$250 (Sponsored by EGI)
- 4th Prize:** \$100 (Sponsored by Chemistry Matters)

Each winner will also receive one of the four books shown below, which have been donated to INEF 2018 by the authors/editors (thanks to Ellen Spears, Gwen O'Sullivan, Robert Morrison and Brian Murphy).



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Litigation Support
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Social Activities

INEF 2018

NIGHT AT THE MUSEUM

Join us on **Monday Evening (June 25th)** for a private reception at the Natural History Museum of Utah (NHMU), sponsored by Waters. Utah State Paleontologist Dr. James Kirkland will talk about a different type of Environmental Forensics: unraveling the history of the earth during the Jurassic and Cretaceous periods. Jim will discuss vertebrate paleontology in Utah (including the famous *Utahraptor*), and will perhaps lead a tour or two of the museum.

The reception will take place after dinner at the Heritage Center, and will include light snacks, desserts, and beverages. It will also include private access to the museum galleries, including the dinosaur exhibits. NHMU is located less than 1 mile from the INEF conference venue, so delegates (who choose to) may hike to the reception after dinner, or take a shuttle bus that will be departing the Guest House at regular intervals, beginning at 18:30.



Dr. James Kirkland, with *Utahraptor ostrommaysorum*

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About NHMU

The Natural History Museum of Utah is housed at the beautiful Rio Tinto Center, a unique 163,000 square foot building, clad in 42,000 square feet of standing seam copper. The museum occupies a prominent place at the edge of Salt Lake City and the University of Utah.

NHMU emphasizes the North American Great Basin and Colorado Plateau, but it also includes material from throughout the world. Exhibits include the dinosaurs of Past Worlds and Utah's archaeological history in First Peoples. The terrace just off of the 5th floor reception area offers a stunning view of Salt Lake City from high up on the east-bench of the Great Salt Lake Valley.

TUESDAY, JUNE 26, 2018: Saints and Sinners. Ice Cream Social and Downtown SLC Pub Crawl.

On Tuesday night, after dinner at the Heritage Center, INEF delegates will gather at the Officer's Club for a typically wholesome Utah activity: an Ice Cream Social. After dinner, those that are interested will depart on light rail (Trax) for a downtown Salt Lake pub crawl, including a scavenger hunt and trivia game. A prize will be awarded to the winner at the closing ceremonies on Wednesday afternoon.



Ice Cream Social and Pub Crawl

Meals / Reception Schedule

The following meals and receptions will be held, and are included as part of your INEF registration. Breakfast is not provided by INEF, but if you are staying at the University Guest House, they offer a free breakfast for guests of the hotel.

MONDAY, JUNE 25, 2018

10:30 -11:00	Morning Coffee/Tea (North Room)
12:20-13:20	Lunch (Heritage Center)
14:40 -15:20	Afternoon Break/Poster Sessions (North Room)
17:00-18:30	Dinner (Heritage Center)
18:30-21:30	Waters Welcome Event (NHMU)

TUESDAY, JUNE 26, 2018

10:30-10:50	Morning Coffee/Tea (North Room)
12:30-13:30	Lunch (Heritage Center)
14:50-15:20	Afternoon Break/Poster Sessions (North Room)
17:00-18:30	Dinner (Heritage Center)
18:30-20:30	Ice Cream Social (North/West Rooms)

JUNE 27, 2018

10:30-10:50	Morning Coffee/Tea (North Room)
12:30-13:30	Lunch (Location: TBA)

MONDAY, June 25, 2018	
8:00 - 9:00	REGISTRATION - Fort Douglas Officer's Club
Plenary Session - Fort Douglas Officers Club - South Conference Room	
8:30 - 8:45	Welcome and Introduction Gwen O'Sullivan, INEF Secretary, INEF 2018 Co-Chair, Mt. Royal University, Canada
8:45 - 9:00	Orientation: The University of Utah and Conference Overview Glenn Johnson, INEF 2018 Chair, University of Utah, USA
9:00 - 9:45	Big Data Visual Analysis Chris Johnson, Distinguished Professor of Computer Science, University of Utah
9:45 - 10:30	Isotopes and Environmental Forensics Thure Cerling, Distinguished Professor of Biology and Geology & Geophysics, University of Utah
10:30 - 11:00	COFFEE/REFRESHMENT BREAK – Fort Douglas Officers Club - North/West Conference Room
BREAKOUT SESSIONS	
	South Conference Room Session 1: Isotope Forensics 1 (p. 13) Moderator: Paul Philp
	East Conference Room Session 2: Data Analysis and Visualization (p. 14) Moderator: Mike Bock
11:00 - 11:20	Isotope Forensics of Perchlorate Neil Sturchio, University of Delaware, Newark, DE, USA
11:20 - 11:40	Evidence Recorded in Fingernails: Carbon, Oxygen, and Strontium Isotopes Reveal Diet and Travel Histories Christy Mancuso, University of Utah, Salt Lake City, UT, USA
11:40 - 12:00	Expanding the Framework for Natural Attenuation Assessments of Chromium Through the Use of Isotopes Jun Lu, Hefei University of Technology, China
12:00 - 12:20	Isotopic Identification of Chlorinated Solvent Sources: Potential Pitfalls in Using Carbon-Chlorine Cross-Plots Farrukh Mohsen, Princeton HydroGeo LLC, Cranbury, NJ, USA
12:20 - 13:20	Visualization of Chemometric Methods in Budd Inlet, WA Will Hafner, NewFields, Edmonds, WA, USA
11:20 - 11:40	Study on Identification Index of Environmental Damage of Hazardous Waste Contaminated Sites Yuanxun Zhang, Univ. Chinese Acad. Sciences, Beijing, China
11:40 - 12:00	Reconstructing Fate and Transport Using Moss Data Steve Mudge, Norwegian Institute for Air Research, Norway
12:00 - 12:20	Integrated Application of RSIMCA, tSNE, and PVA for Chemometric Mapping of PCDD/F Congeners Robert Barrick, Infinity Solutions Group, Seattle, WA, USA
LUNCH – HERITAGE CENTER	
	South Conference Room Session 3: Isotope Forensics 2 (p. 16) Moderator: Neil Sturchio
	East Conference Room Session 4: Multivariate Fingerprinting Methods (p. 18) Moderator: Glenn Johnson
13:20 - 13:40	The Evolution and Future of Stable Isotopes in Environmental Forensics Paul Philp, University of Oklahoma, Norman, OK, USA
13:40 - 14:00	Advances in oil spill forensic using biomarkers and isotope ratio technique. Harry Behzadi, SGS North America, Rutherford, NJ, USA
14:00 - 14:20	Isotopic Reconnaissance of an Urban Water Supply System Yusuf Jameel, University of Utah, Salt Lake City, UT, USA
14:20 - 14:40	Stable Isotopes - A Tool for Traceability and Fraud Detection Thuan Chau, Isoforensics, Inc., Salt Lake City, UT, USA
13:20 - 13:40	Emerging Statistical Methods for Source Apportionment Mike Bock, Ramboll, Portland, Maine, USA
13:40 - 14:00	Determination of Sources of Organic Pollutants and Trace Elements in the Environment Erik R. Christensen, University of Wisconsin-Milwaukee, USA
14:00 - 14:20	Examining Uncertainty Associated with Positive Matrix Factorization Source Apportionment Models Court Sandau, Chemistry Matters, Alberta, Canada
14:20 - 14:40	Challenges and Considerations of Using Disparate Datasets in Multivariate Forensic Analysis Nicholas Rose, TIG Environmental, New York, NY, USA
COFFEE/REFRESHMENT BREAK - Poster Session	
	South Conference Room Session 5: Fate & Transport (p. 19) Moderator: Steve Mudge
	East Conference Room Session 6: Human & Ecological Exposure (p. 21) Moderator: Daniel Mendoza
15:20 - 15:40	Fingerprinting dust from desert playas to the Wasatch Front, Utah Michael Goodman, Brigham Young University, Provo, UT, USA
15:40 - 16:00	Applying a "Hard Science" Disciplined Approach to Identify and Verify Chemical Properties for Safe Response, Handling, and Disposal Cliff Holland, Spill Management Inc., Stoney Creek, ON, CA
15:40 - 16:00	Characterization of PCBs and Mercury Fate and Transport in the Berry's Creek Estuary Todd Martin, Integral, Salt Lake City, Utah, USA
15:40 - 16:00	Spatial Differences in Fine Particulate Matter Exposure across the Salt Lake School District: Dust Event, Inversion, and Ozone Studies Daniel Mendoza, University of Utah, Salt Lake City, USA
16:00 - 16:20	Use of Analytical Contaminant Fate and Transport Modeling in Forensic Source Evaluation Gregory Schnaar, Daniel B. Stevens & Assoc., Silver Spring, MD, USA
16:00 - 16:20	Background Levels of PCDD/Fs, dIPCBs and PXDD/Fs in sera of pregnant Ghanaian women Pennante Bruce-Vanderpuije, University of Buffalo, USA
16:20 - 16:40	Successful Use of Visual Forensics at a Smelter Site Melanie Edwards, Exponent, Bellevue, WA, USA
16:20 - 16:40	Physiological Responses of Chinese Cabbage to Pyrene Stress in Three Growth Periods Yuxian Liu, University of Chinese Academy of Sciences, Beijing, China
16:40 - 17:00	Volatilization and Atmospheric Transport of Chlorpyrifos and Chlorpyrifos Oxon under Field Conditions Supta Das, University of Otago, New Zealand
16:40 - 17:00	An Untargeted Exposure Study of Small Isolated Populations Adam Ladak, Waters Corporation, Milford, MA, USA
17:30 - 18:30	DINNER – HERITAGE CENTER
18:30 - 21:30	Waters Welcome Event at the Natural History Museum of Utah

TUESDAY June 26, 2018		
8:00 - 9:00	REGISTRATION - Fort Douglas Officer's Club	
Plenary Session - Fort Douglas Officers Club - South Conference Room		
8:45 - 9:00	Introduction and Overview of Day 2 David Megson, INEF 2018 Co-Chair, Manchester Metropolitan University, UK	
9:00 - 9:45	Airborne PCBs released from Aroclor and Non-Aroclor Sources in Indoor Environments Keri Hornbuckle, University of Iowa, Iowa City, Iowa, USA	
9:45 - 10:30	PCB Contamination in Anniston, Alabama: A Social History Ellen Griffith Spears, University of Alabama, Tuscaloosa, AL, USA	
10:30 - 10:50	COFFEE/REFRESHMENT BREAK – Fort Douglas Officers Club - North/West Conference Room	
BREAKOUT SESSIONS		
	South Conference Room Session 7: PCBs (p.24) Moderator: David Megson	East Conference Room Session 8: Oil Spill Forensics (p. 26) Moderator: Court Sandau
10:50 - 11:10	PCB Deposition to Glacier Surfaces on Svalbard Mark Hermanson, Hermanson & Assoc. Minneapolis, MN USA	PAH Apportionment at a Site with Severely Weathered Crude Oil Deborah Chiavelli, Anchor QEA, Woodcliff Lake, NJ, USA
11:10 - 11:30	Open Book, Open Source: Chronicling PCB Usage in Book Adhesives Jeffrey Parker, Pacific Groundwater Group, Seattle, WA, USA	Forensic PAH Fingerprinting Techniques and Source Apportionment for Oil Spills Court Sandau, Chemistry Matters, Calgary, AB, Canada
11:30 - 11:50	Bottle Liquid-Liquid Extraction (BLLE) for the economical extraction of PCBs from challenging wastewater samples Brendon A. Parsons, Los Alamos Natl. Lab., NM, USA	Weathering Effects onto Source Identification of Diesel Fuel Contaminated Soils Colin S. Chen, Kaohsiung Normal University, Taiwan
11:50 - 12:10	Understanding PCB Processing in Biota Using Factor Analysis Lisa Rodenburg, Rutgers, New Brunswick, NJ, USA	PAHs in Urban Background: Ratios and Patterns David Mauro, Meta Environmental, Fairport, NY, USA
12:10 - 12:30	Evaluation of dendrochemistry as a novel environmental monitoring tool: The temporal and spatial delineation of persistent organic pollutants Gwen O'Sullivan, Mt. Royal University, Calgary, AB, Canada	Following Traces of Biodegradation Using Thermal Fingerprints. Jun Lu, Hefei University of Technology, China
12:30 - 13:30	LUNCH – HERITAGE CENTER	
	South Conference Room Session 9: PCB and PCDD/F Congener Analysis (p. 28) Moderator: Mark Hermanson	East Conference Room Session 10: Metals (p. 29) Moderator: Gwen O'Sullivan
13:30 - 13:50	How Many PCBs Are There In The Environment And Where Do They Come From? David Megson, Manchester Metropolitan Univ., UK	Evaluating the Source(s) of Metals and Metalloids in Reservoir Sediments – Geogenic or Anthropogenic? Mark Sorensen & Jeff Hess, Gilbane, Concord, CA, USA
13:50 - 14:10	CongenerR: A Tool for Comparing PCB-Congener Data with Different Co-elution Patterns Koshlan Mayer-Blackwell, Pacific Groundwater Group, Seattle, WA, USA	Application of Pine Needles as Bioindicators of Trace Metals in Urban Air Kevin Hayes, Mt. Royal University, Calgary, AB, Canada
14:10 - 14:30	A PCDD/F fingerprint study using the 190 nontoxic congeners: first results Carlo Monti, TIG, Pregassona, Lugano, Switzerland	Record of Lead Pollution in Great Salt Lake Sediments Lihai Hu, University of Utah, Salt Lake City, UT, USA
14:30 - 14:50	A Matlab Tool for Visual Goodness-of-Fit Evaluation in Multivariate Analysis of PCB and PCDD/F Congener Data Glenn Johnson, Univ. Utah, Salt Lake City, UT, USA	Implementation of Circular Economy in Treatment of Landfill Leachate Vedansh Gupta, University of Utah, Salt Lake City, UT, USA
14:50 - 15:20	COFFEE/REFRESHMENT BREAK - Posters	
	South Conference Room Session 11: Air Pollution (p. 31) Moderator: Ben Williams	East Conference Room Session 12: Emerging Contaminants (p. 33) Moderator: Ingrid Ericson Jogsten
15:20 - 15:40	NOx Emissions from Switch Yard Locomotives Identified with a Light-Rail Public Transit Platform Logan Mitchell, University of Utah, Salt Lake City, UT, USA	Sources and Sinks of PBDEs in Treatment Plant Sludges İpek İmamoğlu, Middle East Tech. Univ., Ankara, Turkey
15:40 - 16:00	Towards Improved Bioaerosol Source Apportionment and Modelling Assessments Ben Williams, Univ. West England, Bristol, UK	An Investigation of Emerging Contaminants in Wastewater: Characterization and Identification of Benzotriazole Derivatives by GCxGC-TOFMS Kyra Murrell, Penn State University, University Park, PA, USA
16:00 - 16:20	Household Indoor Particulate Matter Measurement Using a Network of Low-Cost Sensors Shruti Hegde, University of Utah, Salt Lake City, UT, USA	Microbial binding of perfluoroalkyl substances (PFASs) Ingrid Ericson Jogsten, Orebro University, Sweden
16:20 - 16:40	Rigorous Use of a Conceptual Site Model to Guide Development of Multiple Lines of Evidence at Vapor Intrusion Sites Steve Luis, Blayne Hartman, Ramboll, Irvine, CA, USA	The effects of dilution on biodegradation of pharmaceuticals and metagenomics analysis: implication for environmental risk assessment Simone Bagnis, Plymouth University, UK
16:40 - 17:00	AQandU Project: evaluation of a low-cost air quality sensor network in the Wasatch front, United States Tofigh Sayahi, University of Utah, Salt Lake City, UT, USA	Identification and Quantification of Trace Level VOCs in Highly Contaminated Air Samples Heidi C. Hayes, Eurofins Air Toxics, Folsom, CA, USA
17:30 - 19:00	DINNER – HERITAGE CENTER	
19:00 - 21:00	Saints and Sinners / Ice Cream Social and Downtown SLC Pub Crawl	

WEDNESDAY June 27, 2018		
8:00 - 8:45	REGISTRATION - Fort Douglas Officer's Club	
Plenary Session - Fort Douglas Officers Club - South Conference Room		
8:45 - 9:00	Day 3: Introduction and Overview Stephen Mudge, Chairman, International Network of Environmental Forensics	
9:00 - 9:45	A Decade of Environmental Forensic Investigations Related to Shale Gas Exploration – What's Been Learned? Frank L. Dorman, Penn State University, University Park, PA, USA	
9:45 - 10:30	Admissibility And Use Of Environmental Forensics In The Courtroom Jeffery L. Caufield, Esq., Caufield and James, LLP, San Diego, CA, USA	
10:30 - 10:50	COFFEE/REFRESHMENT BREAK – Fort Douglas Officers Club - North/West Conference Room	
BREAKOUT SESSIONS		
	South Conference Room Session 13: Forensics in Litigation (p. 35) Moderator: Michael Wade	East Conference Room Session 14: Emerging Analytical Methods (p. 37) Moderator: Alina Muscalu
10:50 - 11:10	Centredale Manor Superfund Site – A Litigation Case History Graham Ansell, Integral, Annapolis, MD, USA	Developing Forensic Tools to Evaluate the Results of Non-targeted Chemical Analysis Kirk O'Reilly, Exponent, Bellevue, WA, USA
11:10 - 11:30	The Peer Reviewed Literature and the Litigation Process Urs Furrer, Esq. Harriton & Furrer, Armonk, NY, USA	Changes to Polychlorinated Biphenyl PCB Signatures and Enantiomer Fractions in Different Tissue Types David Megson, Manchester Metropolitan Univ., UK
11:30 - 11:50	No Smoking Gun? Environmental Forensic Methods to Still Build a Winning Case Emily Vavricka, Orange, CA, USA	Online monitoring of VOCs from waste effluent by GC-FID and GC-TOFMS Matthew Edwards, SepSolve Analytical, Peterborough, UK
11:50 - 12:10	Environmental Remediation Study Design: Thinking Through to a Forensic/Litigation End Michael J. Wade, Wade Research, Marshfield, MA, USA	Nuclear Magnetic Resonance: An Improved Source Fingerprinting Analytical Tool Julie Konzuk, Geosyntec Consultants International, Toronto, ON, Canada
12:10 - 12:30	Using Thermodynamics to Identify an Atmospheric PCB Source Mark Hermanson, Hermanson & Assoc. Minneapolis, MN USA	Identifying and Quantitating Non-target Environmental Pollutants by using a Routine Comprehensive Two-dimensional Gas Chromatography Method Alina Muscalu, Ministry of the Environment and Climate Change, Toronto, ON, M9P 3V6, Canada
12:30 - 13:30	LUNCH (Location TBA)	
13:30 - 14:30	Closing Ceremonies and Student Paper Awards INEF Committee	

Posters		
West Conference Room		
Monday June 25 to Tuesday June 26 (p. 39)		
	Exposure detection of a variety of pharmaceuticals and personal care products in domestic reclaimed wastewater reuse practices, in Northern Utah Leila Ahmadi, Utah State University, Logan, UT	Characterization of Community Urban Air Quality Using Trees as Biomonitors Kevin Hayes, Mt. Royal University, Calgary, AB, Canada
	Hexabromocyclododecane (HBCDD) Biodegradation in Anaerobic Sediment Mesocosms İpek İmamoğlu, Middle East Tech. Univ., Ankara, Turkey	Assessment of Ecological Risk of Heavy Metals in Farmland: A Case Study in China Yuxian Liu, Univ. of Chinese Acad. of Sciences, Beijing, China
	Method optimization and validation of comprehensive multidimensional gas chromatography using response surface methodology for the application of ignitable liquid residue analysis Nadin Boegelsack, University of Saskatchewan, Saskatoon, SK, Canada	Dual-Channel GCxGC-FID for Routine TPH Analyses Matthew Edwards, SepSolve Analytical, Peterborough, UK
	Advances in oil spill forensic using biomarkers and isotope ratio technique. Harry Behzadi, SGS North America, Rutherford, New Jersey	Recent trends in analytical methods for the determination of PCBs Thomas Tennant, Manchester Metropolitan University, Manchester UK

PLENARY ABSTRACTS

MONDAY, JUNE 25, 2018 - SOUTH CONFERENCE ROOM

9:00 – 9:45

BIG DATA VISUAL ANALYSIS

Chris Johnson*¹

¹Distinguished Professor, School of Computing
University of Utah, Salt Lake City, Utah

* Presenting Author

We live in an era in which the creation of new data is growing exponentially such that every two days we create as much new data as we did from the beginning of mankind until the year 2003. One of the greatest scientific challenges of the 21st century is to effectively understand and make use of the vast amount of information being produced. Visual data analysis will be among our most important tools to understand such large and often complex data. In this talk, I will present state-of-the-art visualization techniques, including ways to visually characterize associated error and uncertainty, applied to Big Data problems in science, engineering, and medicine.



Dr. Chris Johnson is a Distinguished Professor of Computer Science and founding director of the Scientific Computing and Imaging (SCI) Institute at the University of Utah. He also holds faculty appointments in the Departments of Physics and Bioengineering. His research interests are in the areas of scientific computing and scientific visualization.

In 1992, Dr. Johnson founded the SCI research group, now the SCI Institute, which has grown to employ over 200 faculty, staff and students. Professor Johnson serves on a number of international journal editorial and advisory boards to national and international research centers. He is a Fellow of AIMBE (2004), AAAS (2005), SIAM (2009), and IEEE (2014) and has received multiple research awards including the Governor's Medal for Science and Technology, the Utah Cyber Pioneer Award, the IEEE Visualization Career Award, IEEE Charles Babbage Award, the IEEE Sidney Fernbach Award, and the University of Utah's most prestigious faculty award, the Rosenblatt Prize.

9:45 – 10:30

ISOTOPES & ENVIRONMENTAL FORENSICS

Thure Cerling*¹

¹Distinguished Professor of Biology and Geology & Geophysics, University of Utah, Salt Lake City, Utah

* Presenting Author

Stable isotopes and the more rare radioisotopes are useful for tracing time, processes, and movement. I will discuss how some of the variations in stable and radioisotopes come about, and then how they can be used in forensic studies to give information about time, geographic origin, or movement. Time, geography, local geology, ecology provide information about sample history. Principal examples discussed will be taken from our current research problems.



Dr. Thure Cerling is a biogeochemist at the University of Utah. His work primarily concerns the use of isotopes to study biological and geological processes occurring near the Earth's surface. He has done extensive field work in North America, Kenya, and Pakistan, and other geological and biological studies in Argentina, Australia,

Western Europe, and Antarctica. These studies include cosmic-ray produced isotopes to study geomorphology, chemistry of lakes and lake sediments, stable isotope studies of diet and of soils, isotope forensics, and studies of early hominin environments in Africa. He served for 9 years on the US Nuclear Waste Technical Review Board. He is a member of the US National Academy of Sciences.

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TUESDAY, JUNE 26, 2018 - SOUTH CONFERENCE ROOM

9:00 – 9:45

AIRBORNE PCBs RELEASED FROM AROCLOR AND NON-AROCLOR SOURCES IN INDOOR ENVIRONMENTS

Keri C. Hornbuckle*^{1,2}

Nicholas J. Herkert¹, Jacob C. Jahnke¹, and Rachel F. Marek²

¹ Department of Civil & Environmental Engineering; ²IHR-Hydroscience and Engineering; University of Iowa, Iowa City, Iowa 52242

* Presenting Author

There are important sources of airborne polychlorinated biphenyls (PCBs) in indoor environments. Our laboratory has developed novel techniques for sampling and quantifying airborne PCBs and their sources in air, water, and solids, including consumer products. We have measured elevated concentrations of individual PCB congeners in schools and homes. Here we report on our identification of specific sources using direct measurement of PCB fluxes from indoor sources, and from computational modeling that elucidate the relative importance of Aroclor and non-Aroclor sources of airborne PCBs. Aroclor sources are commonly found in schools and other buildings that were constructed for long lifetimes. In these buildings, Aroclors were used to extend the life of caulking, adhesives, and paint, and to extend the useful lifetime of fluorescent lighting and other electrical equipment. Non-Aroclor sources are also found in schools and often in private homes. Sources of these PCBs include resins used on finished kitchen cabinets, and brightly colored paints. There is strong evidence that modern manufacturing of pigments and polymers produces PCBs inadvertently, some of which are potent neurotoxins and/or endocrine disruptors. Our findings indicate that human exposure through inhalation of indoor air may be as important as our exposure to PCBs through diet. Both Aroclor and non-Aroclor sources are contributing to this hazard.



Dr. Keri Hornbuckle Dr. Keri Hornbuckle is the Donald E. Bently Professor of Engineering and Professor of Civil & Environmental Engineering at the University of Iowa. She is an Associate Editor of the ACS journal, Environmental Science and Technology and an Associate Director of the Iowa Superfund Research Program (NIEHS/NIH). Her research

addresses the sources, transport, and fate of persistent organic pollutants, including both legacy and emerging pollutants, with special focus on PCBs. A hallmark of her research is the three-pronged approach that includes field, analytical, and modeling work. For over 25 years, she and her collaborators have examined many aspects of chemicals, including emissions, fate and transport, and exposure.

9:45 – 10:30

PCB CONTAMINATION IN ANNISTON, ALABAMA: A SOCIAL HISTORY

Ellen Griffith Spears*¹

¹Associate Professor, New College/Department of American Studies, The University of Alabama, Tuscaloosa, AL 35487

* Presenting Author

Toxic chemical exposures tell a human story. A case in point is Anniston, Alabama, where disproportionate PCB contamination fell squarely on African American and working class white communities near the chemical plant. A city of 24,000 in the Appalachian foothills, Anniston holds the singular distinction as the locale in the U.S. where chemical manufacturers first commercially produced polychlorinated biphenyls. At stake are industrialists' choices, activists' responses, and the impacts on the lives of residents, exposed or not. More than six decades after production began, and nearly two decades after Congress banned PCBs, residents of Anniston learned that their levels of exposure rivaled workplace exposures anywhere in the world. They began tackling questions of systemic race and class inequality as they attempted to uncover and understand the nature of the chemicals, the consequences of exposure, and what this information means for individuals' health. Environmental scientists and engineers as well as medical professionals have been crucial to unraveling these narratives as the residents sought justice in court. How the various players have handled knowledge of chemical exposure—given or withheld—has been critical in assessing and improving public health.



Dr. Ellen Griffith Spears is an associate professor in the interdisciplinary New College and the Department of American Studies at the University of Alabama. Her research is broadly interdisciplinary, combining environmental history with studies of science, technology, and public health. She is principal investigator in the Landscapes of Change

study, which resulted in the book, *Baptized in PCBs: Race, Pollution, and Justice in an All-American Town*, published in 2014 by the University of North Carolina Press. The book has received numerous awards, including the 2015 Francis B. Simkins Prize from the Southern Historical Association, and the 2015 Reed Environmental Writing Award, from the Southern Environmental Law Center. Ellen has spoken on the social costs of pollution around the U.S. and internationally, including at the 6th International PCB Workshop in Visby, Sweden.

WEDNESDAY, JUNE 27, 2018 - SOUTH CONFERENCE ROOM

9:00 – 9:45

A DECADE OF ENVIRONMENTAL FORENSIC INVESTIGATIONS RELATED TO SHALE GAS EXPLORATION – WHAT’S BEEN LEARNED?

Frank L. Dorman^{1*},

Paulina Piotrowski,¹ Benedikt Weggler¹

¹ Department of Biochemistry and Molecular Biology, Penn State University, University Park, PA, USA

* Presenting Author

Over the last decade, there has been considerable interest in gas well drilling into the Marcellus and Utica shale in the Eastern U.S. In states such as Pennsylvania, Ohio and others, there has been a dramatic increase in the development of such wells, but this has not been without controversy. While the gas-drilling industry claims that their processes are completely safe and undamaging to the environment, several environmental groups strongly claim otherwise. Adding to the controversy, the process of hydraulic fracturing of these wells may use various chemicals that are not without concern. The industrial companies claim to self-disclose their formulations, but this is an overstatement, as the exact compositions are not revealed. If drilling or hydraulic fracturing caused some environmental contamination, it would not be easy to determine the source of the contamination due to the lack of disclosure and oversight of the operators. This results in potentially complex environmental forensics analytical method development and sample analysis to determine if a contamination event has occurred, and who the principle polluter may be.

This presentation will address the sampling, sample preparation and analysis of these materials in an effort to develop the chemical compositional understanding of post-drill and/or post-frac fluids so that source identification and source apportionment may be successful in the event of a release. Additionally, this chemical composition may allow for on-site, or near-site bioremediation if the composition is better understood. Various sample preparation strategies will be discussed. GCXGC-TOFMS and GCxGC-HRTOFMS will be used as determinative techniques due to the inherent advantages over other possible approaches, as well as the data reduction tools necessary for communication of findings from these complex analyses. Finally, the analyses surrounding a gas well drilling event will be discussed where it was determined that gas exploration led to impact of a drinking water system.



Dr. Frank Dorman is an Associate Professor in the Department of Biochemistry and Molecular Biology (BMB) at Penn State University. He is also a member of the Graduate Faculty in Biochemistry, Microbiology and Molecular Biology (BMMB), Chemistry (CHEM) and the Programs in Forensics Science (FRNSC), and Biogeochemistry (BGC), at Penn State. Frank’s research interests are in analytical chemistry

methods development, with a focus on environmental forensics, and traditional forensic applications. Prior to joining the faculty at PSU, Frank was at Restek Corporation for 14 years as the Director of Technical Development, and R&D Senior Chemist.

9:45 – 10:30

ADMISSIBILITY AND USE OF ENVIRONMENTAL FORENSICS IN THE COURTROOM

Jeffery L. Caufield^{*1}

¹ Caufield & James, LLP, San Diego, CA, USA

*Presenting Author

Environmental forensics can play a large role in the investigation as to the sources of contaminants as well as determining the responsible party that might have caused the contamination. In many instances the results of the various investigations conducted on and/or around sites identify multiple potential sources of contaminants. Additionally, in many sites there are multiple operators on the property that may have used the same and/or similar chemicals spread over many years. In many instances the parties will advocate to the regulatory agencies arguments regarding the source and cause of the contamination. In most instances the regulatory agencies decline to make a determination as to the allocation of liability and/or responsibility for the cost to investigate and remediate the underlying contamination and leave that issue up to the Courts to decide. The cost to litigate the issue of the allocation of liability between parties can be very substantial and will often come down to a “battle of the experts.” In many instances both the testifying expert for the trial and even consultant that conducted the investigation may be called as witnesses. In almost every instance a testifying expert can expect his or her opinion to be vigorously challenged and motions filed with the Court to bar their opinion from being introduced at trial. The Federal Courts and various State Court use a widely variable analysis for the admissibility of expert opinions at trial. Both the consultant conducting the investigation and the testifying expert need to understand the standard that may be applied by the Court in analyzing the admissibility of their work and/or opinion in advance. This session will explore the various Federal and State Court admissibility criteria and what both consultants and experts need to understand about the criteria that the Court may apply.



Mr. Jeffery L. Caufield is a partner in Caufield & James LLP. He is a graduate of the University of California Santa Barbara with a degree in environmental studies and worked as an environmental consultant prior to becoming an attorney. Mr. Caufield is a graduate of McGeorge Law School and clerked at the California Department of Fish and Game and the U.S. Department of Interior Regional Solicitor’s office. He has 25 years of

experience in environmental litigation matters including such cases as “Erin Brokovich” and similar matters that have made national headlines. Mr. Caufield has represented parties in well over 100 different contaminant sites in both regulatory enforcement and litigation context. He is on the editorial board of *Environmental Forensics* and routinely publishes articles and lectures on environmental forensics issues.

ORAL ABSTRACTS

MONDAY, JUNE 25, 2018
11:00 – 12:20

SOUTH CONFERENCE ROOM:
SESSION 1: ISOTOPE FORENSICS 1

ISOTOPE FORENSICS OF PERCHLORATE

Neil C. Sturchio*

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* Presenting Author

Perchlorate (ClO_4^-) has both natural and anthropogenic sources. Its widespread presence in the environment and food chain was recognized in the past two decades. Substantial concerns exist about ClO_4^- because of its potentially deleterious effects on human health; the U.S. EPA plans to regulate ClO_4^- in drinking water. Considerable effort has been directed at characterizing the sources and distribution of ClO_4^- in the environment, including ranges in isotopic compositions of Cl and O and their relation to source type, kinetic isotope effects, and isotope exchange. Three principal sources of ClO_4^- have been distinguished by isotopic variation in the environment: (1) synthetic ClO_4^- (manufactured for industrial and aerospace industries); (2) indigenous natural ClO_4^- (interpreted to be largely from atmospheric deposition); and (3) Atacama ClO_4^- (found in natural nitrate-rich salts in the Atacama Desert of Chile and nitrate fertilizers derived therefrom). The natural varieties are distinguishable from each other and from synthetic ClO_4^- because: (1) natural ClO_4^- is enriched in ^{17}O , presumably by photochemical reactions in the upper atmosphere, whereas synthetic ClO_4^- has normal terrestrial mass-dependent ^{17}O abundance (i.e., $\Delta^{17}\text{O} = 0.0 \pm 0.1 \text{‰}$); (2) Atacama ClO_4^- is highly depleted in ^{37}Cl ($\delta^{37}\text{Cl} = -20$ to -10‰); and (3) indigenous natural ClO_4^- has anomalously high ^{36}Cl abundance relative to common Cl in rocks and near-surface fluids. Plants do not fractionate ClO_4^- isotopes relative to water source, and human urine has ClO_4^- isotopic composition reflecting cumulative dietary source(s). Further experimental and theoretical study could lead to more complete understanding of the mechanisms that generate observed natural ClO_4^- isotopic variations. The current database of ClO_4^- isotopic variations has proven useful in identification of the source(s) of dissolved ClO_4^- in groundwater at numerous locations.

EVIDENCE RECORDED IN FINGERNAILS: CARBON, OXYGEN, AND STRONTIUM ISOTOPES REVEAL DIET AND TRAVEL HISTORIES

Christy J. MANCUSO^{1*} and James R. EHLERINGER¹

¹ University of Utah, Dept. Biology, Salt Lake City, UT 84112
* Presenting Author

The purpose of this study was to determine if fingernail isotopes could be used for reconstructing geolocation histories and to examine the convergence in fingernail stable isotope ratios by a non-resident group to that of a resident group following their arrival to Salt Lake City, UT (SLC). The fingernail stable isotopes of residents defined an isotope baseline used to make comparisons with the non-resident population. This study examined stable isotope biomarkers of fingernail clippings from

a resident ($n = 26$) and non-resident ($n = 22$) population in SLC from 2015-2016. We analyzed fingernail clippings for both dietary ($\delta^{13}\text{C}$ and $\delta^{15}\text{N}$) and drinking water inputs ($\delta^{18}\text{O}$ and $\delta^2\text{H}$), with a subset analyzed for geologic signatures ($\text{Sr}^{87}/\text{Sr}^{86}$). In addition, we highlight isotope travel patterns between two volunteers, residents of SLC who traveled to the Galapagos, Ecuador before returning home.

When initial fingernail $\delta^{18}\text{O}$ and $\delta^2\text{H}$ values of non-residents were correlated with precipitation isotopes of their prior locations, regression analyses revealed significant relationships that were similar in the proportion of drinking water inputs into fingernail isotopes as were previously observed in the keratin from hair in individuals from the USA and Asia. Turnover in fingernail stable isotopes of non-residents occurred as they settled into SLC. Resident and non-resident fingernail isotopes were indistinguishable after 71 – 90 days. Mean $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ values of non-residents were not significantly different from the resident population. For those non-residents with fingernail $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ values different from the mean SLC resident values, the values had converged by the conclusion of the study. We found that $\text{Sr}^{87}/\text{Sr}^{86}$ values changed within 4-5 weeks of arrival to SLC. This rapid shift suggests that the $\text{Sr}^{87}/\text{Sr}^{86}$ signal is primarily coming from bathing waters as an exogenous input, as opposed to inputs from dietary and drinking water sources.

Two volunteers who traveled to the Galapagos, Ecuador exhibited interesting patterns. Fingernail $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ values did not exhibit significant changes in their over the course of the study; nor were there differences associated with their time abroad. The $\delta^{18}\text{O}$ and $\delta^2\text{H}$ values shifted and displayed patterns consistent with their reported travel history. We found that $\delta^{18}\text{O}$ and $\delta^2\text{H}$ values were similar to SLC residents when the volunteers resided in the area and as they moved to their new locations there was an isotopic shift. Isotope turnover was rapid and 95% equilibration was estimated after ~50-60 days. $\text{Sr}^{87}/\text{Sr}^{86}$ isotope ratios displayed similar patterns to our non-resident population.

Our findings suggest that $\text{Sr}^{87}/\text{Sr}^{86}$ values reflect an individual current location, while $\delta^{18}\text{O}$ and $\delta^2\text{H}$ values represent the location where the fingernail tissue was developed. This finding further supports the use of fingernail tissues for travel history reconstruction for forensic and homeland security functions.

EXPANDING THE FRAMEWORK FOR NATURAL ATTENUATION ASSESSMENTS OF CHROMIUM THROUGH THE USE OF ISOTOPES

Jun Lu^{1*} and Lucas Hellerich²

¹School of Resources and Environment, Hefei University of Technology, Hefei 230009, China

²Lucas Hellerich, AECOM, Rocky Hills, CT 06067, USA

*Presenting Author

At chromium contaminated sites, quantification of fate and transport in groundwater systems, including natural attenuation processes and source identification, are important parts of the site characterization. The most stable states of chromium in the environment are trivalent chromium [Cr(III)] and hexavalent chromium [Cr(VI)]. Between these two states, the one of environmental concern is Cr(VI) due to its high toxicity. Cr(VI) fate and transport assessments and source issues are typically dealt with by integrating information from natural background, site history, and site geology, hydrogeology and geochemical conditions. Often, past assessments of chromium fate and

transport and monitored natural assessments have relied on evaluation of geochemistry and reductive capacity within groundwater aquifers. Recently, however, there appears to be an increasing use of stable isotopes to provide an additional line of evidence to identify potential sources and to evaluate natural attenuation processes, a component of chromium fate and transport.

This presentation provides a case study involving two sites where groundwater has been contaminated with Cr(VI), one in Connecticut (Site A) whose aquifer was polluted by electroplating solutions between 1930 and 1995, and another in New Jersey (Site B) whose aquifer was polluted by soluble chromium-processing wastes between 1911 and 1963. Over forty groundwater samples were collected from both sites for chromium isotope analysis. In addition, along the predominant migration paths, other relevant parameters were also analyzed including pH, dissolved oxygen (DO) content, oxidation-reduction potential, total chromium and Cr(VI), dissolved organic carbon, ferrous iron [Fe(II)], and divalent manganese [Mn(II)] concentrations. The results show significant enrichment of Cr53 over Cr52 by reduction of Cr(VI) to Cr(III) and influencing factors including concentration of Cr(VI) and dissolved organic carbon and age of the releases. Most interestingly, some findings appear to be inconsistent with those of previous studies including negative correlation between concentrations and Cr53 enrichment and preference of anaerobic conditions for Cr(VI) reduction. The findings from this study provide an additional aspect to consider within the overall framework for evaluation of chromium fate and transport processes, including natural attenuation, at chromium impacted sites.

ISOTOPIC IDENTIFICATION OF CHLORINATED SOLVENT SOURCES: POTENTIAL PITFALLS IN USING CARBON-CHLORINE CROSS-PLOTS

Brian L. Murphy, Exponent, Brandon FL and
Farrukh Mohsen*, Princeton HydroGeo LLC, Cranbury, NJ
* Presenting Author

Carbon and chlorine isotopes can be used to identify sources. The most direct way to do this is to reconstruct the original undegraded isotope values using Rayleigh's Equation. An advantage of this method is that a standard deviation can be computed for the carbon isotope original value estimate. A second method involves using cross plots to demonstrate a consistent relationship between carbon and chlorine isotope values. However, relying solely on cross plots: (1) can lead to data with different Rayleigh's Equation parameters (e.g. initial isotope values) being misidentified as belonging to a particular spill data, and (2) can lead to some data, for example, carbon isotope data for which there is no corresponding chlorine isotope data, being disregarded. We develop a method to use cross plots even when some isotope data is missing, as in this example. Nevertheless, cross plots are particularly valuable if some chemical data are missing such that the extent of degradation is uncertain.

These remarks are illustrated by a case study. The case study also illustrates how to obtain various isotopic parameters. Finally, the case study contains a result for spill origin that is somewhat surprising given well locations and the direction of groundwater flow, a result illustrating the power of isotopic methods.

EAST CONFERENCE ROOM: SESSION 2: DATA ANALYSIS & VISUALIZATION

VISUALIZATION OF CHEMOMETRIC METHODS IN BUDD INLET, WA

Will Hafner^{1*}, Jonathan Nuwer¹, and Pete Striplin²

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² WA Dept. of Ecology, PO Box 47600, Olympia, WA 98504-7600

* Presenting Author

The goal of environmental forensics is to uncover patterns in the target data-set that would otherwise go unnoticed using more conventional analysis. Multivariate statistical methods (chemometrics) are often viewed as the centerpiece of forensics and are frequently given an oversized role both during analysis and when presenting the results. While these methods and their statistical output may represent the foundation of chemometrics, they alone can't tell the full story. Proper visualization of the model output is a key part of maximizing the analysis and presenting the results in a manner that is interpretable by the target audience. We have conducted three sediment dioxin/furan chemometric studies at former wood processing sites in the Puget Sound. This abstract focuses on Budd Inlet near the city of Olympia, WA. Budd Inlet is a large, well mixed embayment with nearly 500 dioxin/furan samples. Source identification and potential source unmixing was performed using a multivariate curve resolution-alternating least squares (MCR-ALS) algorithm. Visualization tools such as Geographical Information Systems (GIS) were used extensively to help interpret the statistical output and display the final results.

Our analysis revealed that the Budd Inlet data-set consisted of three unique dioxin/furan source-types, contributing nearly 98 percent of the total variance across the Inlet. The three profiles were correlated to the following upland sources: 1) hog fuel boiler emissions, 2) pentachlorophenol from historical wood treatment, and 3) polychlorinated biphenyls. The percent contribution of these sources to each sediment sample was mapped spatially (Figure 1), demonstrating the distribution of each source in a way that could be compared to historical operations within the Inlet.

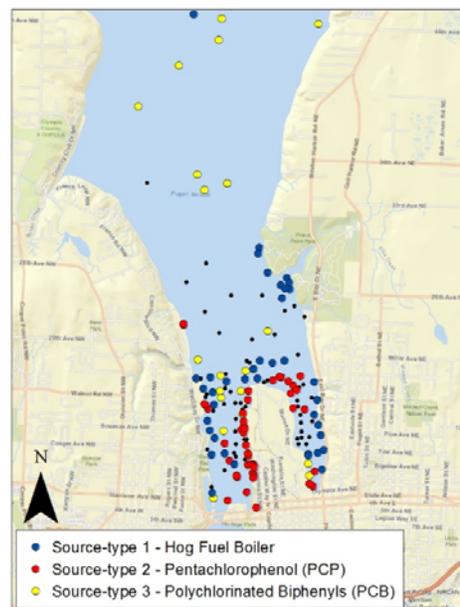


Figure 1. Spatial distribution of source-types

STUDY ON IDENTIFICATION INDEX OF ENVIRONMENTAL DAMAGE OF HAZARDOUS WASTE CONTAMINATED SITES

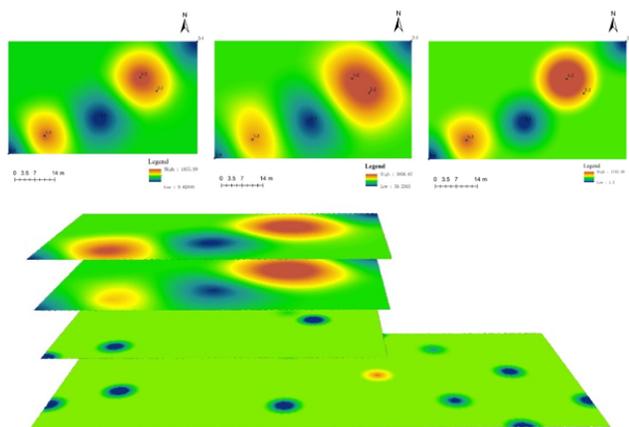
Yuanxun Zhang*, Sumin Chen, Reza Bashiri Khuzestani, and Jinxi Hua, Jing Shang

College of Resources and Environment, University of Chinese Academy of Sciences, Beijing, China

*Presenting Author

Hazardous waste is considered as one of the most critical pollution sources and the contaminated sites could cause detrimental effects on both ecological security and public health. Contaminated sites with hazardous wastes are the trickiest type among all due to the complexity and uncertainty of such systems. Hence, it has long been a challenge for Environmental Damage Assessment technicians to investigate or diagnose the condition of the contaminated sites with hazardous wastes, let alone to make evaluations. Some pollutant species could cause more risks to the ecosystems just with small variations in forms or properties. As a result, only the quantitative chemical analysis is not sufficient to provide a versatile ecological impact assessment. In this research, we proposed an integrated analysis method that combines both quantitative chemical analysis and biological toxicity assay, which can reveal the condition of the contaminated sites directly and intuitively due to its tractability and quantifiable characteristics.

A contaminated site polluted by hazardous wastes was selected which account for a large proportion of environmental damage in judicial practice, based on the analysis method for semi-volatile compounds in soil. Geological and hydrological conditions of the soil environment were investigated, and the concentrations of organics in the soil were analyzed. The results showed various types of contaminants, including pesticides and some Chlorinated Aliphatic Hydrocarbons (CAHs). Some specific organic species (i.e. 1-Piperidinepropanamine, 2-methylpiperidine, di isooctyl phthalate (DEHP), and p-trifluoromethoxyaniline (a pesticide intermediate)) were selected as priority control pollutants based on their high concentrations and risks. Spatial distribution patterns were evaluated using the inverse distance weighted interpolation (IDW) method. Meanwhile, we have established a set of bio-toxicity diagnosis of soil in organic contaminated sites (i.e. the light-emitting loss of in *Photobacterium Phosphoreum* as an evaluation index). Considering the applications of diagnostic methods, the combined biological toxicity diagnosis and chemical analysis, is capable of making comprehensive evaluations for the pollution status of soil body in the contaminated sites. Furthermore, the spatial interpolation of chemical analysis and toxicity diagnostic evaluation methods were performed individually to establish a three-dimensional spatial distribution characterization surfaces. Using the interpolated pollutant concentrations and the luminescence inhibition rates, ARCGIS was used to define the different potential contaminated areas and quantify the land that need to be remediated.



RECONSTRUCTING FATE AND TRANSPORT USING MOSS DATA

Stephen M Mudge*¹, Katrine Aspmo Pfaffhuber² and Hilde Uggerud²

¹ Norwegian Institute for Air Research (IMPACT) and ² Norwegian Institute for Air Research (MILK)

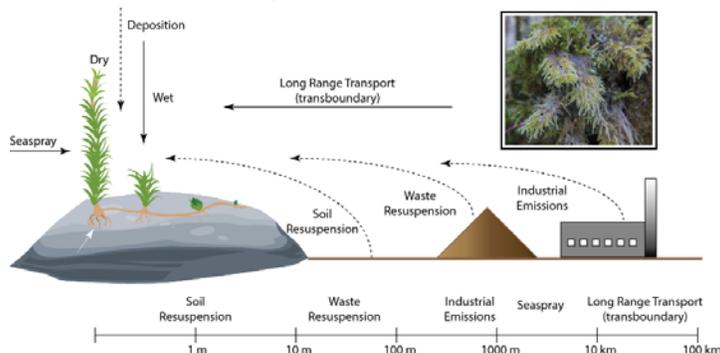
*Presenting Author

Moss samples have been collected across Norway as part of an air monitoring campaign since 1977. The whole scheme has been organised by Eiliv Steinnes since its inception. Since 1990, samples have been collected every 5 years from around 460 sites with over 50 metals analysed in each sample. The analytical technology has changed through time with neutron activation analysis in the early years to high resolution ICP-MS today. Steinnes has published several papers on the change in concentration of selected elements with time. The work presented here takes the same datasets and conducts multivariate statistical analyses to examine the number of different sources that are likely to be impacting the mosses.

One of the advantages to using moss samples is that there is no uptake through a root system and they will only trap airborne particles. However, there are a number of potential sources of the airborne particles including soil splash, short-range transport from local industries or waste tips and long-range (transboundary) transport. PCA, PLS and PVA were all applied to the data and a number of examples of sources and their pathways identified. PVA suggests that there are too many sources to make sense of the whole dataset in one go and so some of the elements were excluded on the basis of their ability to be predicted within a sensible number of sources. By reducing the elemental cohort to smaller number of variables, four major sources types become apparent in the data across the years.

There are two obvious long-range transport signatures that enter into Norway (a) from Europe to the south of the country and (b) from the Russian mining town of Nikel. With regard to the first source, all of the typical anthropogenically enhanced metals such as Pb, Zn and Cu characterise this signature. The second of these transboundary sources emanates from the nickel extraction town of Nikel just over the border in Northern Russia. Using the metal signature from particles collected in air filters at Svanvik on the Norwegian side of the border, a PLS model was constructed to determine the extent that this signature can explain the moss data. In this case, the signal from Nikel could be traced 450 km into Norway. Unexpectedly, two other sites at other locations within Norway also had a high explained variance from this signature. At both of these sites, there are metal processing industries.

There are signatures related to the distance from the sea using the Na / K proxy for the marine influence and a second signature related to altitude. The distance between sample sites is necessarily quite large (20+ km) in order to cover the whole country and this means that gradients away from local sources where the path length is small might be missed. However, a number of sites stand out using the elemental data and all of these are related to either on-going or historical mineral extraction and processing.



INTEGRATED APPLICATION OF RSIMCA, TSNE, AND PVA FOR CHEMOMETRIC MAPPING OF PCDD/F CONGENERS

Mark Jonathan Cejas^{1†} and **Robert C. Barrick**^{1*}

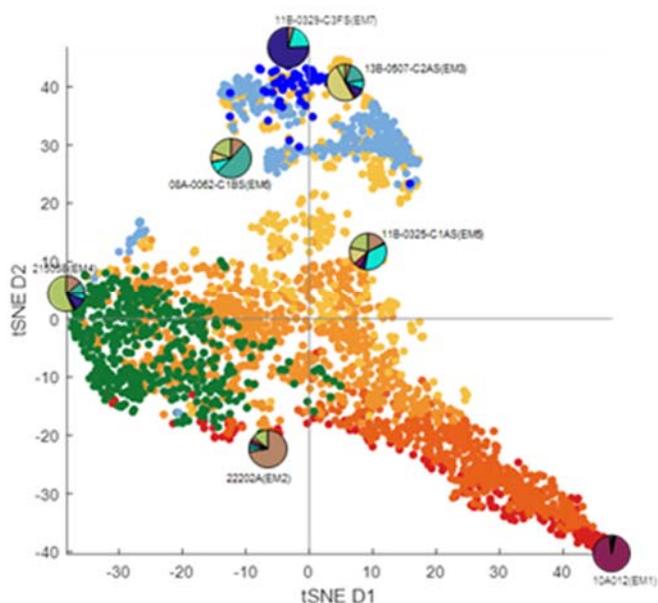
¹ Infinity Solutions Group, 12565 42nd Ave NE, Seattle, WA
98125

[†] Currently with Pace Analytical

* Presenting Author

Unique distributions of the 17 toxic polychlorinated dibenzodioxin and dibenzofuran (PCDD/F) congeners used in risk assessments are the basis for distinguishing major sources in sediment environments. We apply Robust Independent Modeling of Class Analogy (RSIMCA) to classify over 2,800 river sediment samples into seven “clusters” or as outliers to all clusters after an initial screening of a 3,255 sample dataset. This multivariate statistical output is compressed from seven latent dimensions into two interpretable dimensions using t-Distributed Stochastic Neighbor Embedding (tSNE) graphics. Polytopic Vector Analysis (PVA) is then used to identify distinct source end-members based on PCDD/F characteristics of the classified samples.

Among several advantages, the integrated chemometrics approach a) applies emerging data visualization tools in this “Big Data” era to retain the fidelity of high-dimensional data attributes of a chemical dataset spanning over two decades of sample collection; b) employs a classification technique undisturbed by compositional outliers yet tracks those for subsequent investigations; c) provides an intuitive reduced-dimensional data visualization map for the PVA mixing polytope solution; d) fills a data gap in the contextual inventory of PCDD/F source dynamics in a complex river system; and e) serves as a backdrop for further forensics investigations of the finer structure of less dominant point sources and potential upland source end-members in sediments. This tiered chemometrics strategy provides a strong weight-of-evidence approach to the interpretation of sediment data.



MONDAY, JUNE 25, 2018
13:20 – 14:40

SOUTH CONFERENCE ROOM: SESSION 3: ISOTOPE FORENSICS 2

THE EVOLUTION AND FUTURE OF STABLE ISOTOPES IN ENVIRONMENTAL FORENSICS

R. Paul Philp¹

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* Presenting Author

Environmental forensics has come a long way in the past four decades. In my opinion the development of modern environmental forensics paralleled the development of analytical techniques such as GC, GCMS and slightly later GCIRMS. There was of course a long history of forensic investigations for over 100 years prior to these developments but few of those investigation focused on environmental cases. In the 1970s when these early developments were taking place, many of the more conventional EPA methods were also being developed and became very popular in environmental studies and remain so today. But from a forensic point of view (who did it??) the EPA methods are of little use since they were primarily designed for monitoring compounds of interest in the environment and looking for changes in concentrations of such compounds. Such an approach will rarely indicate who was responsible for the release.

In this talk it is proposed to illustrate, with examples, how environmental forensics has developed over the years and how it will continue to evolve over the coming years. Since the 1970s the basic techniques being used have not changed a great deal. Yes sensitivity of the instruments has improved, improved methods of separation have been developed but the key to improving the effectiveness of environmental forensics is a better understanding of the origin and history of the products being investigated. For example in investigations related to petroleum products there are many unique trace components that are powerful for distinguishing products that have long been known by the petroleum geochemists but rarely used in the environmental arena. Similarly with chlorinated solvents for example, a knowledge of the manufacturing process say for PCE would instantly make one aware of the futility of trying to use stable isotopes to determine the manufacturer of a sample of PCE. These are but two examples but a knowledge of such small details are one of the keys to the continued successful application of the forensic approach to environmental cases.

ADVANCES IN OIL SPILL FORENSIC USING BIOMARKERS AND ISOTOPE RATIO TECHNIQUE

Harry Behzadi, Ph.D¹

¹SGS, VP of Business Development North America

* Presenting Author

Determination of parties liable or guilty in order to recover costs of the cleanup and remediation, has grown dramatically in last decade, environmental forensics has emerged as a discipline directed toward this goal. Traditionally, these studies have been addressed through utilization of techniques such as gas chromatography (GC) and gas chromatography–mass spectrometry (GCMS). Biomarkers play a very important role in characterization, and source identification in environmental

forensic investigations of oil spills. Biological markers or biomarkers are one of the most important hydrocarbon

groups in petroleum for chemical fingerprinting. Relative to other hydrocarbon groups in oil such as alkanes and most aromatic compounds, biomarkers are more degradation-resistant in the environment. Also biomarkers formed under different geological conditions and ages may exhibit different biomarker fingerprints. Biomarkers can be detected in low quantities in the presence of a wide variety of other types of petroleum hydrocarbons by the use of the gas chromatography/mass spectrometry (GC/MS). Chemical analysis of environmental samples for biomarkers generates great information to environmental forensic investigations in terms of determining the source of spilled oil. This is achieved by differentiating and correlating oils, and monitoring the degradation process and weathering state of oils under a wide variety of conditions.

In recent years, stable isotopes, primarily determined through the use of combined gas chromatography–isotope ratio mass spectrometry (GC-C-IRMS), have emerged as an equally important tool in environmental forensics. Determination of stable isotopes is not new, having been around for over 50 years. The ability to determine the isotopic composition of individual compounds in complex mixtures is relatively new and came about with the development and commercial availability of combined gas chromatograph–isotope ratio mass spectrometers (GC-C-IRMS) in the late 1980s and early 1990s. Combined approach of using biomarkers and isotope ratio can lead to accuracy and confidence of the forensic conclusion of the results. As we will see in the presentation in some cases the GC-C-IRMS could be the only possible technique for identification. Depending on the samples, GC-C-IRMS can be the only reliable technique for fingerprinting due to lack of biomarkers.

ISOTOPIC RECONNAISSANCE OF AN URBAN WATER SUPPLY SYSTEM

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Public water supply systems (PWSS) are complex distribution systems and critical infrastructure, making them vulnerable to physical disruption and contamination. Exploring the susceptibility of PWSS to such perturbations requires detailed knowledge of the supply system structure and operation. Although the physical structure of supply systems (i.e., pipeline connection) is usually well documented for developed cities, the actual flow patterns of water in these systems are typically unknown or estimated based on hydrodynamic models with limited observational validation.

Here, we present a novel method for mapping the flow structure of water in a large, complex PWSS, building upon recent work highlighting the potential of stable isotopes of water (SIW) to document water management practices within complex PWSS. We sampled a major water distribution system of the Salt Lake Valley, Utah, measuring SIW of water sources, treatment facilities, and numerous sites within in the supply system. We then developed a hierarchical Bayesian (HB) isotope mixing

model to quantify the proportion of water supplied by different sources at sites within the supply system. Known production volumes and spatial distance effects were used to define the prior probabilities for each source; however, we did not include other physical information about the supply system. Our results were in general agreement with those obtained by hydrodynamic models and provide quantitative estimates of contributions of different water sources to a given site along with robust estimates of uncertainty. Secondary properties of the supply system, such as regions of “static” and “dynamic” source (e.g., regions supplied dominantly by one source vs. those experiencing active mixing between multiple sources), can be obtained from the results.

The isotope-based HB isotope mixing model offers a new investigative technique for analysing PWSS and documenting aspects of supply system structure and operation that are otherwise challenging to observe. The method could allow water managers to document spatiotemporal variation in PWSS flow patterns, critical for interrogating the distribution system to inform operation track contaminants, optimize water supply and monitor, and enforce water rights.

STABLE ISOTOPES - A TOOL FOR TRACEABILITY AND FRAUD DETECTION

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*Presenting Author

Stable isotopes of H, O, C, N, S, and Sr have been widely used in the field of anthropology, biology and ecology to characterize dietary behaviors and regionality. In recent years, isotope signatures have been applied to traceability and fraud detection of commercial goods as well as reconstruction of travel history of decedent to help shed light on cold case investigations. Other isotopes of interest are boron, lithium and chlorine isotopes; used to characterize fluid dynamic and transport. With the growing interest to use isotope analyses, it is essential to understand the current limitations associated with analytical procedures and data interpretation to better utilize isotopes as a tool for traceability and fraud detection.

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EAST CONFERENCE ROOM:

SESSION 4: MULTIVARIATE FINGERPRINTING METHODS

EMERGING STATISTICAL METHODS FOR SOURCE APPORTIONMENT

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* Presenting Author

Multivariate chemical fingerprinting utilized the differences in the chemical profiles of chemicals such as PCBs PAHs and dioxins for different sources. If multiple sources come in the environment simple visual methods are often inadequate to determine what the sources are and their contributions. Receptor modeling and statistical unmixing represent tools that are designed to address question regarding (1) the chemical composition of each source or fingerprint and (2) the contribution of each source or fingerprint to each sample. These questions are often addressed using chemical mass balance (CMB) and positive matrix factorization (PMF). The implementation of these specific methods in EPA tools, and therefore the unofficial endorsement of these methods by EPA, contributes to their popularity. Glenn Johnson (Johnson et al 2014 and previous editions) compared PMF with other receptor modeling methods (e.g. PVA, ALS, TTFA, etc.) and found that these methods provide comparable results during testing. However, new methods based on recent advances in pattern recognition, data analytics, and Bayesian analysis might also be readily applied to statistical unmixing.

In this paper we present the evaluation of a number of alternative methods for statistical unmixing that include: simple least squares mixing models, nonnegative matrix factorization (NMF), blind source separation (BSS), and Bayesian methods. The assumptions, data requirements, difficulty of implementation, and the ability to correctly unmix a known mixture for each method were evaluated. The results show remarkable consistency in the results obtained using these different methods but also reveal that these methods exhibit certain advantages and disadvantages. For example, Bayesian methods show particular promise in characterizing variability and uncertainty in both the source profiles and the source contributions in individual samples while also providing a means to incorporate prior knowledge. Some methods appear to be more robust to missing data and outliers. In most cases these new tools do not have a demonstrable advantage over the traditional tools but Bayesian methods seem to show promise for additional development.

DETERMINATION OF SOURCES OF ORGANIC POLLUTANTS AND TRACE ELEMENTS IN THE ENVIRONMENT

Erik R. Christensen*

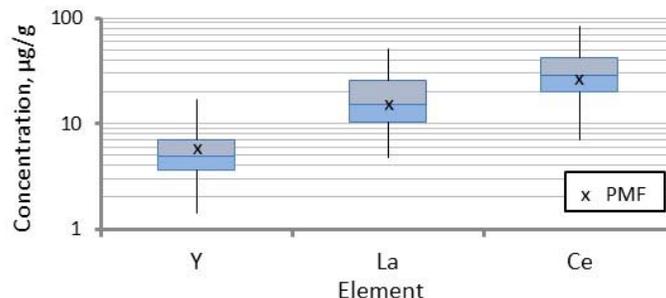
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* Presenting Author

Source apportionment of organic pollutants can be carried out by chemical mass balance (CMB) modeling if sources, but not contributions, are known. Both sources and contributions may be determined by factor analysis with nonnegative constraints

(FNCC) or positive matrix factorization (PMF). Combining a Bayesian CMB model with PMF yields probability distributions of source contributions. We review here results for polycyclic aromatic hydrocarbons (PAHs) in sediments from Lake Calumet, Illinois (FNCC) and Illinois River (CMB-PMF). PMF results for polychlorinated biphenyls (PCBs) in sediments of the Sheboygan River, Wisconsin, and for polybrominated diphenyl ethers (PBDEs) in sediments from six water bodies in Arkansas are also discussed along with recent PMF results for trace elements in moss and soil in Norway.

Major PAH sources in Lake Calumet and the Illinois River are coke oven, traffic, coal and wood combustion. Results from Sheboygan River indicate the original Aroclor 1248, 1254 mixture from Tecumseh Co., and anaerobic dechlorination profiles. Results for PBDEs in an Arkansas wastewater retention pond near Albemarle Co. reflect factors (1) deca-BDE, (2) octa/deca-BDE, (3) penta/deca-BDE with debromination, (4) penta/deca-BDE, and (5) deca with debromination. Sediment dating demonstrate that factor 2 was dominant from 1952 to 1989 consistent with timing of the receipt of wastewater effluent. Results for trace elements in soil of Norway show that the rare earth element Y:La:Ce ratio in soil is consistent with literature data for grazing lands.



Box plot of Y, La, Ce concentrations in grazing land soils in Norway compared with relative PMF element loadings of factor 2, normalized to lanthanum, La.

EXAMINING UNCERTAINTY ASSOCIATED WITH POSITIVE MATRIX FACTORIZATION SOURCE APPORTIONMENT MODEL

Court D Sandau^{1,2*} Lacey Harbicht¹, Phil Richards¹, Khalid Lemouji²

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*Presenting Author

Many contaminated sites and superfund sites have mixed plumes or mixtures of contaminants of concern from multiple potential sources. Examples of mixed plumes could include mixed free phase petroleum plumes (e.g. condensate) or polycyclic aromatic hydrocarbons (PAHs) from crude oil spills mixing with upstream background sources or local anthropogenic sources (storm water runoff) of PAHs in sediments.

Although multivariate statistical analysis such as principal component analysis and hierarchical analysis provide insight on potential end members and likely source patterns, they are unable to determine the amount of each of the contributing sources in each of the samples (source apportionment).

Positive matrix factorization can be used to determine the number and chemical fingerprints of the sources of contaminants present on the site. In addition, these statistical

tools can also apportion the amount of contaminants in each sample, thereby allowing liability to be distributed according to the chemistry of the contaminants and those responsible for the release. Apportionment is important for litigious cases as it allows the calculation of who should pay for what portion of the cleanup. When the cost of the cleanup is high, even small percentage responsibilities can be worth millions of dollars which raises questions about the uncertainty around apportionment percentages assigned to samples and potentially responsible parties.

This presentation will use real case studies as well as experimental mixtures to explore the uncertainty associated with PMF source apportionment and potential methods to define the uncertainty so that results can be relied upon and better understood for legal proceedings.

Lawyers, regulators and environmental professionals involved in superfund sites, spill monitoring and liability determination will find this presentation educational in how these statistical models are able to determine sources and amounts of those sources of contaminants on site and potential address the uncertainty that accompanies these models.

Brief biography

Court D. Sandau, Ph.D., P.Chem. is the principal of Chemistry Matters Inc. and is an adjunct professor at Mount Royal University. Dr. Sandau's technical expertise includes analytical and environmental forensic chemistry, toxicology, and risk assessment.

CHALLENGES AND CONSIDERATIONS OF USING DISPARATE DATASETS IN MULTIVARIATE FORENSIC ANALYSIS

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Multivariate forensic methods can be useful in the allocation process for identifying contaminant sources and apportionment of costs between sources. However, data are rarely collected with quantitative or semi-quantitative forensic methods in mind as data are often collected by multiple entities for different purposes over long time spans. Moreover, historic sources may no longer be present or may be in various stages of remediation. In these cases, using the data for a purpose outside of the original intent of the data ("secondary use") is often necessary or may be the only cost-effective option. The quality of the data, including analytes measured and detection limits, can vary based on differences on the entities collecting and analyzing the samples. Thus, combining such data for secondary use in multivariate forensic analyses requires careful consideration of the usability and harmonization across datasets to draw valid conclusions from the data. When evaluated carefully with an understanding of secondary use issues, the combined dataset can provide useful insights that would otherwise be unobtainable. In this paper we present approaches for evaluating and utilizing such disparate datasets, with real-world examples.

MONDAY, JUNE 25, 2018

15:20 – 17:00

SOUTH CONFERENCE ROOM: SESSION 5: FATE & TRANSPORT

FINGERPRINTING DUST FROM DESERT PLAYAS TO THE WASATCH FRONT, UTAH

Michael Goodman¹, Gregory CARLING¹, Diego FERNANDEZ²,
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* Presenting Author

Dry lakebeds (playas) are important dust sources globally, with potentially harmful impacts on downwind urban areas. The Wasatch Front (population >2 million) in northern Utah, USA, is located adjacent to multiple playas, including the Great Salt Lake (GSL). As water levels on GSL continue to decline due to drought and water diversions, there could be intensified dust emissions from the newly exposed lakebed. To quantify fluxes from GSL relative to other playas, we developed geochemical and isotopic fingerprints of dust sources and compared them to dust deposition along the Wasatch Front. Dust emissions were sampled at GSL and seven playas in western Utah, including Sevier Dry Lake, and dust deposition was sampled at four locations in the Wasatch Front, including Provo, Salt Lake City, Ogden, and Logan. All dust samples were analyzed for mineralogy, bulk chemistry, ⁸⁷Sr/⁸⁶Sr and other isotope ratios on multiple leachate fractions. Sr isotope (⁸⁷Sr/⁸⁶Sr) ratios in the carbonate mineral fraction was variable in the playa dust sources, ranging from 0.7100 in Sevier Dry Lake to 0.7150 in GSL. Wasatch Front dust deposition samples fell within these endmember values, ranging from 0.7110 to 0.7130. Using ⁸⁷Sr/⁸⁶Sr ratios and elemental concentrations, we developed a mixing equation to quantify seasonal fluxes from GSL and Sevier Dry Lake to the Wasatch Front. Using ⁸⁷Sr/⁸⁶Sr and the U/Sr ratios, GSL contributed ~10% to ~50% of the dust flux along the Wasatch Front in Fall 2015. GSL was a less important dust source in Spring 2016, contributing ~0% to ~15% of the total dust flux. These findings suggest that elemental concentrations and ⁸⁷Sr/⁸⁶Sr of carbonate minerals may be useful for evaluating dust emissions from playas worldwide, and that ⁸⁷Sr/⁸⁶Sr measurements should not be restricted to the silicate fraction for dust provenance studies.

CHARACTERIZATION OF PCBs AND MERCURY FATE AND TRANSPORT IN THE BERRY'S CREEK ESTUARY

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* Presenting Author

Background/Objectives. Polychlorinated biphenyls (PCBs) and mercury are contaminants of potential concern (COPCs) at the Berry's Creek Study Area (BCSA) Superfund Site. The BCSA is a side embayment of the Hackensack River estuary in the meadowlands of New Jersey, and includes over 1,000 acres of intertidal marshes and waterways. Tidally-driven interaction

of the marshes and the waterways has considerable influence on the physical and chemical structure of the system. The expansive marshes generate a substantial amount of organic matter, which influences COPC fate and transport through adsorption, particulate resuspension and deposition, and other processes. Characterization of these processes is important to understanding current and future risks posed by the site and to providing a framework for remedial alternatives analyses.

Approach/Activities. An investigation was completed in 2014 and 2015 involving collection of surface water samples for laboratory analysis and in situ optical measurements to support continuous, high temporal resolution quantification of COPC concentrations over one to two month-long periods. The study involved collection of data at fixed locations in the main channel of BCSA and in several marsh tributaries. Current velocities and other ancillary parameters were recorded concurrent with the optical measurements to evaluate COPC responses to tidal flows and in response to storm events. The data collected from the investigation were evaluated in conjunction with other data sets to support an understanding of COPC fate and transport in BCSA.

Results/Lessons Learned. COPC concentrations in surface water are closely linked to interactions of particulates with the surface of waterway sediment bed as a result of routine particulate resuspension and deposition processes. High organic content particulates deposit to the surface of the sediment bed during low velocity (e.g., slack tides, neap tides) periods and adsorb COPCs while in contact with the sediment bed. Resuspension of these particulates during peak tidal velocities and storm flows, in turn, brings COPCs into the surface water column where they are available for exposure and transport. Monitoring of the marsh tributaries demonstrates a consistent net flux of particulate PCBs, mercury, and methyl mercury mass into the marshes as suspended particulates in the flooding tide are retained within the marshes. This process results in a net exchange of particulate COPC mass from the surface of the waterway sediment to the marshes; thereby slowing the rate of natural recovery of the marshes. Further, while there is a significant net flux of methyl mercury (dissolved plus particulate) moving into the marshes, a small mass of dissolved methyl mercury (10% of total) is exported out of the marshes during ebb tide.

USE OF ANALYTICAL CONTAMINANT FATE AND TRANSPORT MODELING IN FORENSIC SOURCE EVALUATION

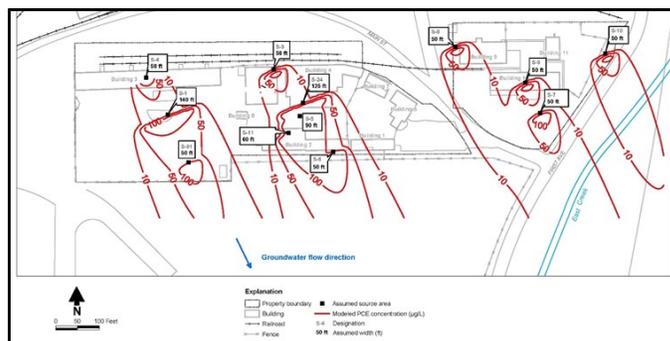
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Forensic environmental investigations often have the objective of determining the source and timing of contaminant releases to soil and/or groundwater. To this end, quantitative analyses are often conducted to evaluate the present pattern of environmental contamination against possible release scenarios. For example, a typical question is "can the present extent of a known groundwater plume be possible with a release that occurred in a specific year?" Hydrogeologic contaminant fate and transport models are often used as a component of this determination, and range in sophistication from simple one-dimensional travel time calculations to advanced three-dimensional numerical simulators.

One-dimensional travel-time calculations typically do not account for known physical processes and are often misapplied. On the other end of the spectrum, fully calibrated numerical fate and transport models are in some cases necessary, but can be laborious to develop and have the potential for erroneous results due to gridding and boundary condition issues. Although often over-looked, analytical contaminant fate and transport models simulate several relevant physical processes (e.g., three-dimensional diffusion/dispersion, degradation, sorption), account for various release geometries and scenarios (e.g., plug release versus continuous source), can be implemented in common spreadsheet or simple coding programs, and are often appropriate for evaluating known contaminant patterns against possible release scenarios. This presentation will focus on several recent case studies of the use of analytical contaminant transport modeling in source evaluation related to groundwater and soil vapor plumes.



SUCCESSFUL USE OF VISUAL FORENSICS AT A SMELTER SITE

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* Presenting Author

Forensic analysis related to smelter sources can be complex despite a short list of contaminants identified at many sites. Lead and arsenic are common among the list of contaminants of concern (COCs) with additional metals identified based on historical details of a particular site. A short list of metals provides very limited information for conducting complex forensic data analysis, with analysis further complicated by the variety of alternative sources for each metal and the natural occurrence of most metals. Because of its unique visual properties when compared to soil, smelter waste or slag can frequently be identified visually more easily than through data analysis methods.

Forensic assessment based on visual inspection of properties near a former smelter site can provide sufficient detail to direct remediation efforts. Successful characterization of smelter waste may require training field personnel on what to look for in sophisticated microscope photos of samples. Alternatively, in this era of data science, electronic image processing of field photographs could automate classification and conclusions while removing an element of subjectivity.

An example case study demonstrates successful use of visual classification and acceptance from regulators for use in targeting remediation decisions. The visual forensic assessment eliminated data analysis (i.e., sampling) and remediation considerations at 35% of properties within the community.

VOLATILIZATION AND ATMOSPHERIC TRANSPORT OF CHLORPYRIFOS AND CHLORPYRIFOS OXON UNDER FIELD CONDITIONS

Supta Das^{1*}, Kimberly J. Hageman^{1,2}, Sue Michelsen-Heath³, Ian Stewart¹, Alison Mercer³

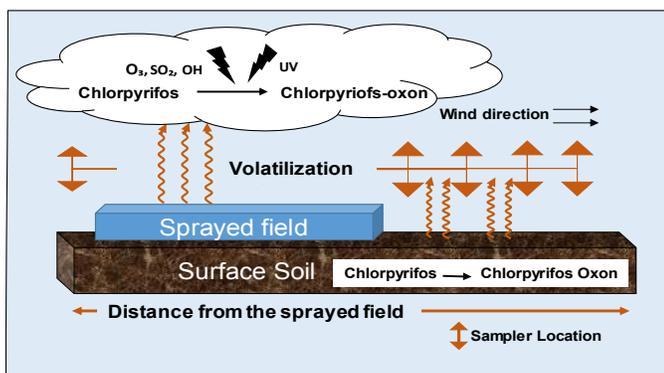
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*Presenting Author

Vapor drift occurs when pesticides volatilize from sprayed fields and are blown off-site by the wind, potentially affecting non-target ecosystems. Organophosphate insecticides can travel many kilometers through the atmosphere and due to their toxic and moderately persistent nature, damage may occur away from the application site. The objective of this work was to better predict the transport and fate of organophosphate insecticide, chlorpyrifos. To this end, we sprayed chlorpyrifos on a field of Purple Tansey (*Phacelia tanacetifolia*) at a farm near Ida valley, Central Otago, New Zealand in January 2017. Seven low volume and one high volume active air samplers were deployed 30 meters to 1 km away from the sprayed field to collect airborne chlorpyrifos and chlorpyrifos oxon for 21 days after spraying. Soil samples were also collected from the same distances throughout the study period. We quantified chlorpyrifos and its oxon in the air and soil samples and used temperature, relative humidity, wind direction and rainfall to understand the concentration trends with time and space. These results can be used to predict distances to which threshold concentrations that cause risk to non-target organisms extend.



Key Words

Organophosphate insecticides, chlorpyrifos, chlorpyrifos oxon, atmospheric transport, air sampling

EAST CONFERENCE ROOM:

SESSION 6: HUMAN & ECOLOGICAL EXPOSURE

APPLYING A "HARD SCIENCE" DISCIPLINED APPROACH TO IDENTIFY AND VERIFY CHEMICAL PROPERTIES FOR SAFE RESPONSE, HANDLING, AND DISPOSAL

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*Presenting Author

Personnel who may have to deal with the uncertain nature and properties of unknown chemicals at an environmental incident, hazardous waste site, industry or in a laboratory need a way to identify the actual risks and hazards they may face. This applies whether the personnel are emergency responders, forensic researchers or waste clean-up crews. There is, however, a quick-check system to identify chemical properties of labeled, unlabeled, unknown or mixed chemicals. The system uses pH paper, starch paper and a source of flame such as a barbecue lighter or Bunsen burner. The basic test takes less than 60 seconds and will identify or verify high-risk properties such as whether substances are oxidizers or reactive to heat, air or water, their range of flammability and their corrosiveness.

The test results provide vital information for responders to make critical decisions, whether dealing with a laboratory spill or a full-scale hazardous material emergency. Using hard science helps in dealing with time-critical issues, such as when, or whether, to add water to modify a chemical reaction when a bad situation could turn into a disaster.

Whether working with laboratory or industrial chemicals or responding to a major emergency, hard science can provide the information needed to Approach the scene, Secure the area, and keep unprotected and unauthorized personnel out. It identifies the physical and chemical properties of known, unknown and newly formed substances and allows personnel to assess the risk, hazards and potential scales of impact including when it is safe to Respond or take other appropriate action.

SPATIAL DIFFERENCES IN FINE PARTICULATE MATTER EXPOSURE ACROSS THE SALT LAKE SCHOOL DISTRICT: DUST EVENT, INVERSION, AND OZONE STUDIES

Daniel L. Mendoza^{1,2*}, Erik Crosman², Logan Mitchell², Alex Jacques², Derek Mallia², Ben Fasoli², John Horel², John Lin², and Robert Paine¹

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* Presenting Author

The Utah Recess Guidance is a set of recommendations developed to protect school children from exposure to poor outdoor air quality, particularly during winter time inversion events when fine particulate matter (PM_{2.5}) is often elevated. The pollutant concentration is read at 8 AM from the nearest Utah Division of Air Quality (UDAQ) sensor and used as a

guideline for whether or not children should be allowed to play outside during recess. There are several problems with this approach. UDAQ air quality data is updated hourly so there is an hour delay in resolving air quality levels that can change quickly. Stationary monitoring is sparse (typically between one to three per county) and therefore cannot resolve spatial variability in outdoor air quality across urban centers. Here we investigate a new method for estimating PM_{2.5} and ozone concentrations at 40 schools in the Salt Lake School District (SLSD) using all available stationary and mobile observation platforms during a dust event on December 20th, 2017 (Figure 2), a winter-time inversion event, and elevated summer ozone.

Our findings strongly recommend a revision to the school recess guidance and further investigation to estimate the association of elevated pollutant levels with student absences.

BACKGROUND LEVELS OF PCDD/Fs, DLPCBs AND PXDD/Fs IN SERA OF PREGNANT GHANAIAN WOMEN

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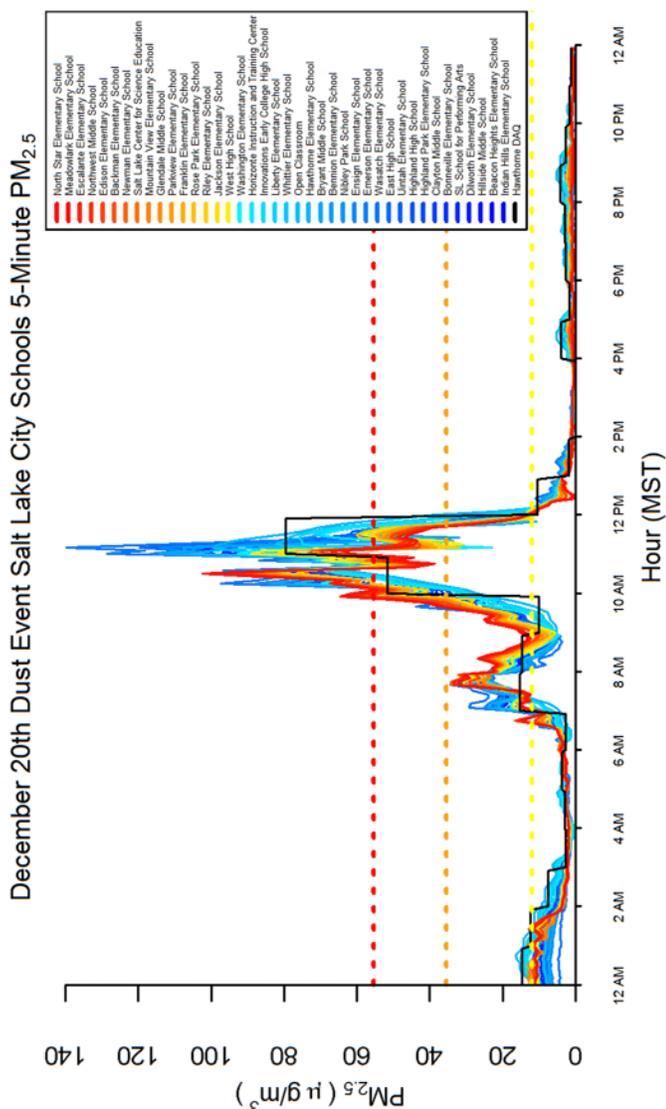
⁶ Environmental Protection Agency, P. O. Box MB 326, Ministries Post Office, Accra, Ghana

* Presenting Author

Vulnerable populations such as pregnant women and their developing foetuses are considered to be at increased risk from exposure to dioxin-related compounds (DRCs). DRCs include polychlorinated dibenzo-p-dioxins and furans (PCDD/Fs), dioxin-like polychlorinated biphenyls (dlPCBs), and polyhalogenated dibenzo-p-dioxins and furans (PXDD/Fs, X=Br or Cl). In regions where associations between exposure levels to DRCs and health risks are identified, the impact of maternal body burdens on foetal exposure becomes significant.

In this study, we investigated the potential sources of exposure on body burdens in maternal serum of 33 primiparous Ghanaians, aged between 18 and 34 years, with no documented exposure to DRCs. The purpose of the study was to provide a reference for background exposure levels of DRCs in sera of pregnant women, to assess the risks from DRCs, and to compare levels obtained with published data.

Approximately 2 g of serum was collected from each participant along with information on participant health, dietary habits, demographic, residential and occupational data. Serum lipids were extracted using C18 SPE with hexane, lipids were cleaned-up with Captiva-EMR lipid removal cartridge. Concentrations of DRCs in serum were determined using GC-APCI-qqMS (Waters, Xevo). The mean concentrations for DRCs were: 2.13 pg/g TEQ PCDD/F WHO-2005 lipid weight (lw) (range: 0.80-5.03 pg/g lw), 0.10 pg/g TEQ dlPCBs WHO-2005 lw (range: 0.01-0.31 pg/g lw), and 6.03 pg/g tentative TEQ PXDD/F WHO-2005 lw (range: 0.96-21.44 pg/g lw). The results indicate that age and dietary intake of seafood and dairy products had a strong influence on PCDD/F and dlPCB levels in serum of pregnant Ghanaian women. Elevated concentrations were also recorded from participants in Accra which may be attributed to open-air burning of domestic, electronic wastes and combustion fumes from vehicular transportation.



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PHYSIOLOGICAL RESPONSES OF CHINESE CABBAGE TO PYRENE STRESS IN THREE GROWTH PERIODS

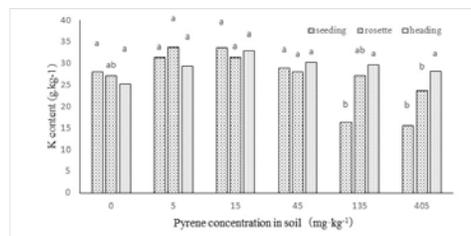
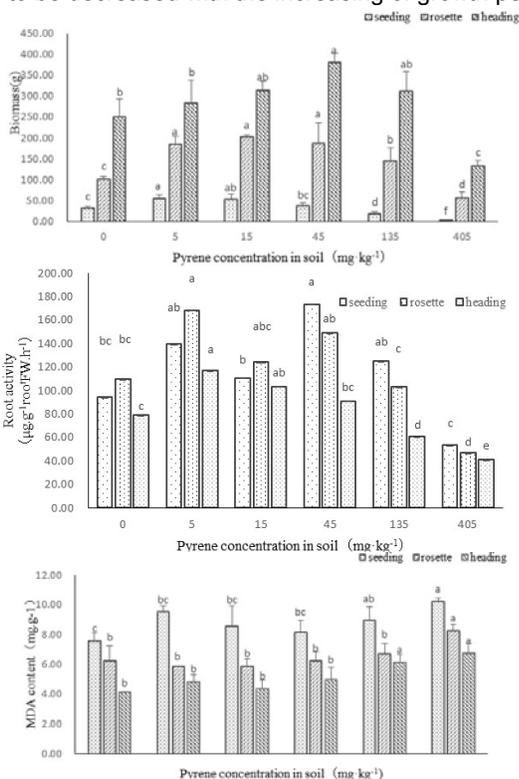
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* Presenting Author

Project supported by: The State Key Research & Development Program of China (2016YF0503604)

To better understand the growth and physiological responses of Chinese cabbage to soil PAHs stress, we investigated biomass, malondialdehyde (MDA) and root activity of Chinese cabbage in three growth periods (the periods of seedling, rosette, and heading). Chinese cabbage were grown in pots with soil treated with various concentrations of pyrene (0, 5, 15, 45, 135 and 405 mg·kg⁻¹). The results showed that the biomass and root activity of Chinese cabbage in three growth periods was increased at first and then decreased with the increasing concentration of pyrene. The biomass was increased by 66.89%, 90.23% and 52.19% respectively at the concentrations of 5 mg·kg⁻¹ pyrene in the period of seedling, 15 mg·kg⁻¹ pyrene in the period of rosette, and 45 mg·kg⁻¹ pyrene in the period of heading, compared with the control, but decreased at the concentration of 405 mg·kg⁻¹ in three growth periods. The concentration of 45 mg·kg⁻¹ increased root activity significantly in the period of seedling. But different results were found that only the concentration of 5 mg·kg⁻¹ pyrene increased root activity by 53.65% and 48.31% at the other two periods. The content of MDA was increased with the increasing time, by 34.61%, 32.48% and 63.37%, respectively at the concentration of 405 mg·kg⁻¹ pyrene in these three growth periods. Compared with the control, the concentration of 15 mg·kg⁻¹ increased potassium content of Chinese cabbage by 19.81%, 16.03% and 31.18% respectively in different growth periods. It was concluded that low concentration of pyrene could increase the biomass of Chinese cabbage, but the pyrene stress to Chinese cabbage tended to be decreased with the increasing of growth periods.



AN UNTARGETED EXPOSURE STUDY OF SMALL ISOLATED POPULATIONS

Adam Ladak*², Pierre Dumas¹, Lauren Mullin², Paul Goulding³

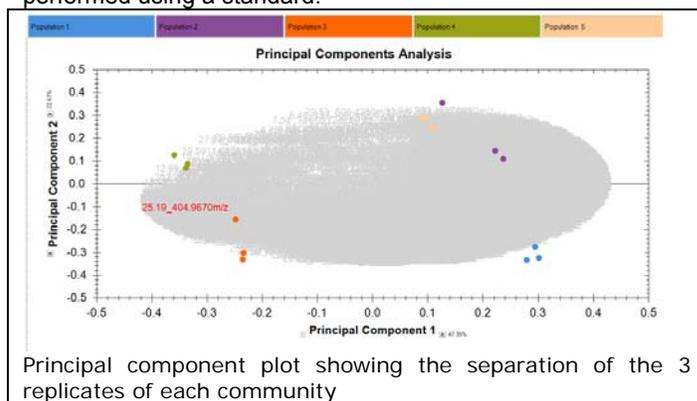
¹ Institut national de santé publique du Québec, QC, Canada

² Waters Corporation, Milford, MA, USA; ³ Waters Corporation, Newcastle Upon Tyne, United Kingdom

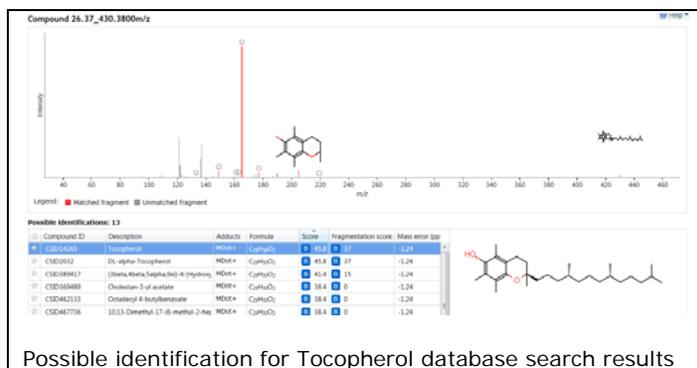
*Presenting Author

In this study pooled plasma samples from individuals living in different small isolated coastal communities were analyzed using an exposomics approach, in order to determine whether differences exist between communities with regard to families and concentrations of contaminants. Samples were analyzed using atmospheric pressure chemical ionization gas chromatography (APGC) coupled to high resolution mass spectrometry (HRMS), operated in data independent acquisition mode, whereby precursor and fragment information were collected in a single run.

First, targeted analysis was performed against a defined contaminants database. Then multi variant analysis (MVA) was carried out to determine any difference between the communities. Elucidation of unknown contaminants was also accomplished with the software which involved searching online databases and matching structural information to the high energy data. Finally confirmation of one of the findings was performed using a standard.



Principal component plot showing the separation of the 3 replicates of each community



Possible identification for Tocopherol database search results

TUESDAY, JUNE 26, 2018
10:50 – 12:30

SOUTH CONFERENCE ROOM:
SESSION 7: PCBs

**PCB DEPOSITION TO GLACIER SURFACES ON
SVALBARD**

Mark HERMANSON¹, Elisabeth ISAKSSON², Camilla TEIXEIRA³
and Derek MUIR³

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² Norwegian Polar Institute, Tromsø, Norway; Environment and
Climate Change Canada, Burlington, Canada

* Presenting Author

During spring 2014, we sampled seasonal surface snow from four glaciers on Svalbard in the eastern Arctic to analyze for 209 polychlorinated biphenyl congeners. This is the first cross-Svalbard snow sampling for analysis of PCBs. Our goal was to identify possible PCB sources. The Kongsvegen site is at elevation 700 m.a.s.l., 78.76° N, 13.34° E; the Holtedahlfonna site is 1150 m.a.s.l. at 79.13° N, 13.27° E, Lomonosovfonna site is 1202 m.a.s.l. at 78.82° N; 17.43° E, and Austfonna is 740 m.a.s.l. at 79.48° N, 24.00° E. All sites are close to each other: The distance between western-most (Hotedahlfonna) and eastern-most (Austfonna) sites is 225 km. Holtedahlfonna is 41.3 kilometers north from Kongsvegen, which is 35.8 km from the nearest town, Ny-Ålesund. Holtedahlfonna and Lomonosovfonna are above the tropospheric boundary layer all year (1000 m.a.s.l. in winter), while Kongsvegen and Austfonna are above the summer boundary layer at 500 m.a.s.l. Considering that the snow samples are winter accumulation, Kongsvegen and Austfonna represent sites within the boundary layer during the snow season.

Results show highest Σ PCB flux = 26.7 pg cm⁻² yr⁻¹ at Kongsvegen, 43% greater than the next highest flux at Holtedahlfonna, 18.7 pg cm⁻² yr⁻¹, and 85% greater than the lowest flux at Lomonosovfonna, 14.4 pg cm⁻² yr⁻¹, similar to Austfonna flux, 15.4 pg cm⁻² yr⁻¹. All sites were dominated by tetrachloro and pentachloro homologues, indicating an influence by long-range atmospheric transport, although at different magnitudes. Air-mass back trajectories were similar for each site, verifying this observation. However, the trichloro homologue contributed more to the western sites than the eastern site at Austfonna, suggesting a stronger source of certain congeners. The dichloro homologue followed a similar but smaller trend. The observation of PCB-5, a non-Aroclor PCB in western samples suggest that a Russian PCB product, Trichlorodiphenyl (TCD) may have been a source, especially to the western sites.

PCB congener profiles for all samples are dominated by PCB-52, PCB-70+74, PCB-95, PCB-101, PCB-110, not always in that order. The Kongsvegen congener profile has a high correlation to Holtedahlfonna, suggesting a similar source of different magnitude. It also has a more diverse number of contributing PCB congeners than Austfonna, suggesting a local source in addition to long-range atmospheric transport.



**OPEN BOOK, OPEN SOURCE: CHRONICLING PCB
USAGE IN BOOK ADHESIVES**

Jeffrey S. PARKER¹, Koshlan MAYER-BLACKWELL²

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98102

* Presenting Author

Polychlorinated biphenyls (PCBs) are a class of synthetic organic chemicals phased out of United States' manufacturing in 1979 due to their environmental persistence and carcinogenic effects. The PCB composition of a variety of industrial products, such as paints, dielectric fluids, and caulks have been well documented (e.g. ITF 1972, Durfee et al. 1976, Erickson and Kaley 2011); however, the specific composition of PCBs in many other common consumer products have been comparatively overlooked. For instance, patents (DuPont 1953), trade journals (Paper Industry 1959), technical literature (Norris and Draghetti in Skeist 1962), and Monsanto internal memoranda (1969 and 1970) identify Aroclors as a plasticizer component in polyvinyl acetate hot melt adhesives for unsewn paperback bookbinding. However, specific PCB formulations, concentrations, and dates of use for these adhesives are not well established. The *Pocket Book* brand pioneered mass-market paperbacks in the United States beginning in 1939 and was an early adopter of hot-melt adhesives. We have assembled a set of *Pocket Book* branded paperback books published between 1939 and 1979. Chemical analysis of the bindings in these production-dated books provides an opportunity to better identify the timing of PCBs used in hot-melt adhesives, and identify potential changes in PCB formulations used for this application over time. This research will (i) inform estimates of PCB content remaining in pre-1979 paperback books housed in homes, stores, and libraries and (ii) indicate whether PCBs are an expected byproduct during the historic and ongoing recycling of paper products containing hot-melt adhesives.

**BOTTLE LIQUID-LIQUID EXTRACTION (BLLE) FOR
THE ECONOMICAL EXTRACTION OF PCBs FROM
CHALLENGING WASTEWATER SAMPLES**

Brendon A. Parsons¹, W. Kirk Hollis¹, Stephen M. Trujillo¹, and
Thomas M. Yoshida¹

¹ Los Alamos Natl. Lab., P.O. Box 1663, Los Alamos, NM 87545

* Presenting Author

The extraction of polychlorinated biphenyls (PCBs) from raw sewer wastewaters is technically challenging due to high amount of suspended solids and tendency to form emulsions, in addition to the presence of large quantities of co-extracted compounds such as hydrocarbon oils and lipids. While several extraction techniques are available for extraction of organic compounds from aqueous matrices, they tend to perform poorly when analyzing samples from sewer systems that combine sanitary and industrial wastewater functions, as is implemented at Los Alamos National Laboratory (LANL). Bottle liquid-liquid extraction (BLLE) is a modification to LLE where the extraction is performed directly in the sample bottle using gentle rolling over long time periods to extract the aqueous phase without forming emulsions. BLLE allows for the unattended simultaneous extraction of up to 40 samples overnight using only a motor-driven bottle roller and the sample bottles as the extraction equipment. After extraction, the organic solvent extract is separated from the aqueous phase and further sample preparation may be performed without modification to clean-up procedures.

This presentation will demonstrate the utility of BLLE for the extraction of PCBs from challenging wastewater samples, along with realized benefits in reducing solvent consumption and improving flexibility versus other extraction techniques. I will also cover novel improvements to BLLE for facile separation of the organic solvent phase and reduction or elimination of drying agents (e.g., anhydrous sodium sulfate) from the process waste stream.

UNDERSTANDING PCB PROCESSING IN BIOTA USING FACTOR ANALYSIS

Lisa RODENBURG^{1*}, Mohammad Mahdi CHITSAZ¹, and Alexandra ANDERSON¹

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* Presenting Author

Fingerprinting of polychlorinated biphenyl (PCB) congener patterns in air, water, and sediment has helped us identify PCB sources in ecosystems across the United States, where all 209 PCB congeners are routinely measured. In these environmental compartments, PCBs from Aroclors retain identifiable fingerprints. In biota, however, fingerprints are more altered, so identifying the PCB source(s) can be challenging. This presentation will discuss the results from fingerprinting of PCB data from both freshwater (Portland Harbor Superfund Site and the Hanford Site, WA) and estuarine systems (the Duwamish River near Seattle, WA as well as the New York/New Jersey Harbor) and across a variety of organisms, including benthic organisms, crabs, fish, osprey eggs, and otter scat. Across these varied species and ecosystems, there are common fingerprints that are similar to Aroclors but have undergone weathering via characteristic absorption, distribution, metabolism, and excretion (ADME) processes. For example, Figure 1 shows how the Aroclor 1260 pattern can change. In some organisms, the fingerprint isolated by positive matrix factorization closely resembles the original Aroclor 1260 (bottom panel), while in other organisms, a fingerprint is isolated that is similar to Aroclor 1260 but shows the characteristic metabolism of PCB 147+149 while PCB 153+168 is not metabolized (i.e. remains abundant; top panel). Co-located sampling demonstrates that spatial patterns of contamination are consistent in both sediment and benthic biota. Otter scat shows unique congeners patterns dominated by four peaks containing congeners that are known to be resistant to degradation (PCBs 83+99, 129+138+160+163, 180+193, and 153+168), which suggest that the alteration of PCB fingerprints in biota is dominated by metabolism, not excretion.

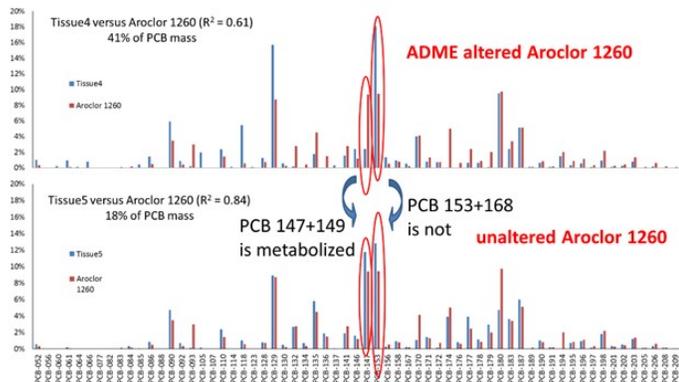


Figure 1. Two PCB fingerprints isolated from benthic biota in the Portland Harbor Superfund Site.

EVALUATION OF DENDROCHEMISTRY AS A NOVEL ENVIRONMENTAL MONITORING TOOL: THE TEMPORAL AND SPATIAL DELINEATION OF PERSISTENT ORGANIC POLLUTANTS

Gwen O'Sullivan¹, David Megson², Eric Reiner³, Xavier Ortiz³

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² Manchester Metropolitan University, Manchester, United Kingdom

³ Ministry of Environment & Climate Change, Toronto, Canada.

* Presenting Author

Alberta is Canada's largest oil and natural gas producer and is home to vast deposits of oil sands. Insufficient monitoring data and a poor understanding of predevelopment conditions make it difficult to quantify the cumulative effects of petroleum development. Measuring historic deposition of pollutants in the environment offers significant promise to increase our understanding of the impacts arising from anthropogenic activity. Dendrochronological methods, including dendroecology and dendrochemistry, have been in use for more than 100 years to provide a record of archaeological and climate events. More recently dendrochemistry has been used to assess the time frame of environmental contamination.

We will present the finding from the analysis of tree cores from a variety of urban, industrial and rural settings in Alberta and examine the temporal persistent organic pollutant loading, both qualitative (e.g., what types of POPs were present) and quantitative (e.g., what were the baseline (pre-industrial) concentrations). The presentation will highlight the potential, and limitations, of tree cores to provide temporal and chemical data that can be used to determine the changing environmental conditions over the lifespan of the sampled trees.

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EAST CONFERENCE ROOM

SESSION 8: OIL SPILL FORENSICS

PAH APPORTIONMENT AT A SITE WITH SEVERELY WEATHERED CRUDE OIL

Deborah Chiavelli^{1*}, Peter Simon², Philip Simon², and Mike Rury¹

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* Presenting Author

We were tasked with quantifying the contribution of residual spilled heavy crude oil from a pipeline breach to surface soil PAH contamination several years post cleanup. Challenges included pre-existing hydrocarbon contamination from background sources and advanced weathering of the crude oil from years of surface exposure.

We present a concentration-based PAH apportionment model robust to a wide range of oil weathering stages and sensitive to small amounts of oil mixed with larger amounts of background PAHs. A notable observation was that 5- and 6-ring PAHs (5+PAHs) were more resistant to weathering than petroleum biomarkers, and despite their relatively low abundance in crude oil, provided a reliable forensic tracer of the crude oil at this site.

Spill area soil, upgradient soil, and crude oil in a range of weathering states were analyzed for PAHs and petroleum biomarkers. The most weathered crude oil reference samples were petroleum tar/surface soil aggregations collected six years post spill.

Conventionally, weathered petroleum is fingerprinted using both petroleum biomarkers, which are resistant to weathering, and ratios of alkylated PAHs with similar weathering rates. The 5+ PAHs, more associated with pyrogenic PAH sources, are rarely used for petroleum fingerprinting due to low abundance and lack of alkylated PAH results. However, biomarkers and alkylated PAH ratios in the petroleum tar samples were too altered by weathering to be used for fingerprinting, whereas 5+PAH in the petroleum tar were relatively unweathered and had a distinct fingerprint from background.

We developed a mixing model series with a range of oil weathering stages based on 5+ PAHs. To increase sensitivity to small amounts of oil, the models included one biomarker and several 4-ring alkylated PAH that were most resistant to weathering in the petroleum tar samples. The models provided an excellent fit to soil samples from the spill area and were used to quantify benzo(a)pyrene concentration attributable to background versus crude oil in site samples.

FORENSIC PAH FINGERPRINTING TECHNIQUES AND SOURCE APPORTIONMENT FOR OIL SPILLS

Court D Sandau^{*1,2} and Phil Richards¹

¹ Chemistry Matters Inc., Calgary, AB,

² Statvis Analytics Inc., Edmonton, AB,

*Presenting Author

Remediation and long term monitoring of oil spills in any environment requires confirmatory analysis to demonstrate the clean-up has achieved its goals and this general involves the monitoring and fingerprinting of Polycyclic Aromatic hydrocarbons (PAHs). However, due to their ubiquitous nature, PAHs generally have confounding issues with sources unrelated to the oil.

PAHs in fish, sediments, and water are not specific for petroleum because there are a range of natural and non-point sources which

can produce considerable concentrations of PAHs. Sources of PAHs that are unrelated to release oil can include forest fires, natural coal exposures and oil seeps, vehicular exhaust and crank case oil drips, and wood preservatives. Distinction of PAHs from a spill can be conducted using environmental forensic techniques, such as PAH fingerprint histograms, PAH diagnostic ratios, or statistical techniques such as Principle Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA). One step further, allows the relative concentration of each source to be determined using source apportionment techniques such as non-negative matrix factorization.

This presentation will describe a case study on how to conclusively determine PAHs resulting from the release of oil into a freshwater river from those occurring from natural or other upstream sources. All the techniques described above were used to provide conclusive and easy to understand graphs and visuals to communicate the identification of the oil related PAHs as well as determine the amount of oil related PAHs that were in the sediment samples. This provided clear communication to the stakeholders and allowed the client to focus remedial activity and plan future monitoring in known areas of higher impacts.

Environmental professionals involved in spill remediation or oil spill monitoring will find this presentation applicable.

Weathering Effects onto Source Identification of Diesel Fuel Contaminated Soils

Colin S. CHEN^{1*}, Chien-Jung TIEN¹, and Chih-Yu Ho¹

¹ Department of Biotechnology, National Kaohsiung Normal University, Kaohsiung 824, Taiwan

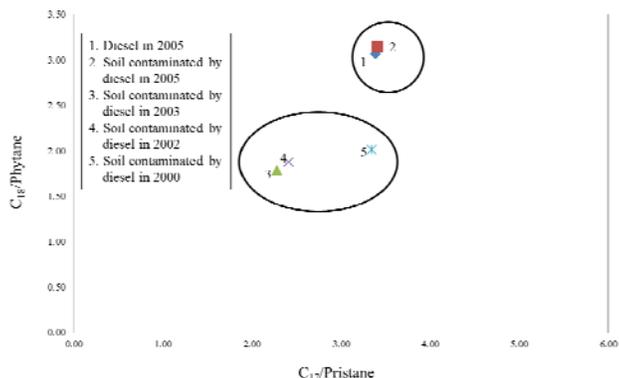
* Presenting Author

The objective of this study was to evaluate weathering effects onto hydrocarbon fingerprinting and distribution patterns of diesel fuels, fuel source screening and differentiation, source-specific marker compounds, and diagnostic ratios of diesel fuel constituents by laboratory and field samples. Aged diesel contaminated soils collected in 2000, 2002, 2003 and 2005, were used for the weathering study. For weathering studies, change of chemical constituent and biodegradation effect of aging diesel contaminated soils were important factors to be considered, especially when there was a prolonged period of weathering processes.

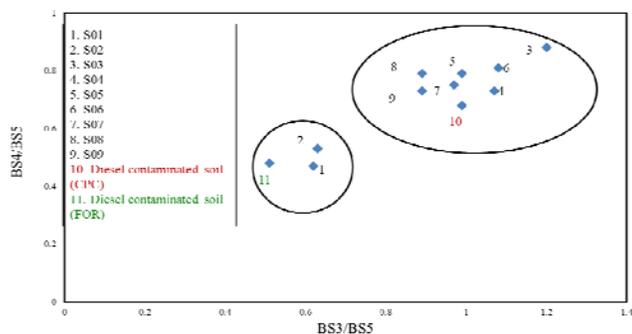
After the long term weathering processes of 11 and 13 years, compounds with molecular weight smaller than C₉ alkanes were disappeared in soils contaminated by diesel fuel in 2003 and 2005, respectively. Also it was found that fuel constituents with molecular weight smaller than C₁₀ alkanes were depleted in diesel contaminated soil of 2002. For soil sample through 16 years of weathering processes, compounds with molecular weight smaller than C₁₁ alkanes were degraded. In contrast to the long term effect, compounds with molecular weight smaller than C₁₂ alkanes were disappeared in soils contaminated by diesel fuels of Chinese Petroleum Company (CPC) and Formosa (FOR) for 365 days of weathering process.

It was evident that Isoprenoids, bicyclic sesquiterpanes (BS) and alkylated PAHs are less susceptible to the effects of biodegradation. The ratios of characteristic factors such as pristane/phytane, C₁₅ sesquiterpane/8β(H)-drimane (BS3/BS5), C₁₅ sesquiterpane/8β(H)-drimane (BS4/BS5), C₁₅ sesquiterpane/C₁₅ sesquiterpane (BS4/BS6), C₁₅ sesquiterpane/8β(H)-homodrimane (BS3/BS10) and 8β(H)-drimane/8β(H)-homodrimane (BS5/BS10), methylphenanthrene Indices (MPI), methyl-naphthalene ratio (MNR), methyl-phenanthrene ratio (MPR) could be adopted as forensic indicators in diesel contaminated sites. The results indicated that the characteristic ratio of diesel fuel produced in 2005 with soils contaminated by diesel fuel of

2005 were similar. Apparently characteristic ratio matched the information sources. Finally, source identification was attempted for samples collected from different fuel contaminated sites by using the unique pattern of sesquiterpanes.



Cross-plots of the diagnostic ratios of C₁₇/Pristane versus C₁₈/Phytane in diesel fuels



Cross-plots of the diagnostic ratios BS₃/BS₅ versus BS₄/BS₅ in diesel contaminated soils

PAHS IN URBAN BACKGROUND: RATIOS AND PATTERNS

David Mauro^{*1}

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* Presenting Author

At INEF 2015, Mr. Mauro presented the results of analyses of tars and tarry materials from former manufactured gas plants, coke plants, tar refineries, and related operations to identify chemical patterns with the greatest forensic value. It was shown how tar formation conditions affect the composition of byproducts of these operations and how the patterns in those byproducts could be used for source identification.

The INEF 2015 presentation focused on strictly pyrogenic, high polycyclic aromatic hydrocarbon (PAH) concentration substances. However, it has long been recognized that PAHs are nearly ubiquitous at low to moderate concentrations in urban surface soils, and that the PAHs generally originated from both pyrogenic and petrogenic sources. Two studies of PAHs in urban surface soil in the United States were completed by META Environmental, Inc. for the Electric Power Research Institute and the Gas Research Institute. Surface soil samples from over 500 sites in 42 population centers in four states were collected and analyzed for PAHs; this represents the most comprehensive study of PAHs in urban surface soil available. The samples were analyzed for GC/FID fingerprints and 40 PAHs and alkylated PAHs by GC/MS.

The chemical data from the background PAH study were “mined” for additional characteristics and compounds and trends that help delineate former manufactured gas plant (MGP)-derived PAHs

from general urban background. The study data indicated that much, if not all, of ambient PAHs in soil are from non-MGP-sources. The findings of the data mining exercise will be summarized and chemical characteristics, such as PAH patterns and co-contaminants, with the greatest forensic value will be highlighted.

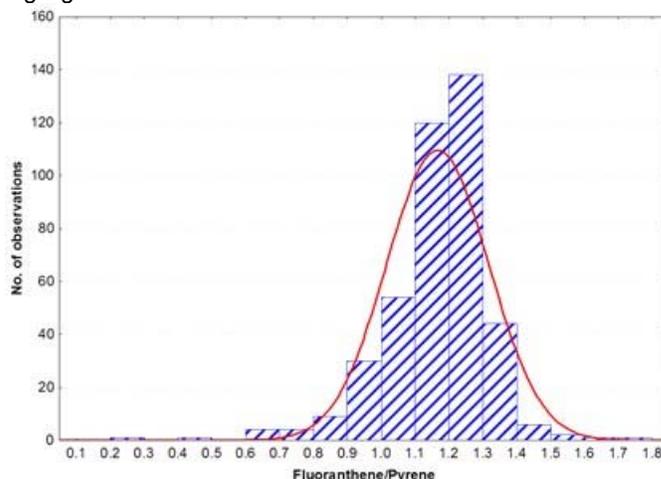


Figure 1. Distribution of Fluoranthene/Pyrene Ratio in 418 Background Soil Samples

FOLLOWING TRACES OF BIODEGRADATION USING THERMAL FINGERPRINTS

JUN LU^{*1}, STEVE GAITO² AND KANGPING CUI¹

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²AECOM, Providence, RI, USA

*Presenting Author

Billions of dollars are spent every year to clean up contaminated sites in the U.S. and around the world. To achieve effective remediation, a sound conceptual site model (CSM) is critical. A CSM integrates many aspects of site information that can be used to guide remediation design. This presentation will focus on the use of the thermal fingerprints (i.e., anomalies) to identify traces of biodegradation at petroleum impacted sites. This method has the potential to cost-effectively quantify light non-aqueous liquid (LNAPL) depletion and to achieve green and sustainable remediation.

It is well known that the biologically mediated processes that destroy hydrocarbons release heat creating temperature anomalies above the natural soil temperature profile. Recent research has focused on measuring temperature in and around LNAPL-affected areas and characterizing thermal fingerprints (areas of warmer temperature) associated with exothermic natural source-zone depletion processes. Thermal fingerprints can be measured in an existing monitoring well network through long-term deployment of data-loggers or instantaneous readings with a thermocouple. This relatively inexpensive data collection can identify where aerobic biodegradation is occurring. A model was constructed to calculate heat flux associated with thermal fingerprints identified in LNAPL source zones and, correspondingly, the rate of hydrocarbon degradation generating the excess heat in the subsurface. Additionally, thermal anomalies at a site with active bioventing were measured by installing data-loggers in a monitoring well and thermistors buried in the ground to demonstrate the applicability of in-well temperature monitoring.

TUESDAY, JUNE 26, 2018
13:30 – 14:50

SOUTH CONFERENCE ROOM:
SESSION 9: PCB AND PCDD/F CONGENER
ANALYSIS

HOW MANY PCBs ARE THERE IN THE
ENVIRONMENT AND WHERE DO THEY COME FROM?

David MEGSON^{*1,2} Rhys JONES³, Glenn JOHNSON⁴,
Thomas BROWN⁵, Courtney SANDAU²

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³ Waters Corporation, Manchester, UK

⁴ University of Utah, Utah, U.S.A.

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* Presenting Author

A significant limitation with some PCB forensic cases is that they use analytical methods that only target a subset of specific PCBs. There can be a huge variation in the PCBs targeted by different methods with many established to focus solely on co-planar PCBs (e.g. WHO 12) to assess human health risks, or on PCBs that are abundant in Aroclors (e.g. i7 & i3 PCBs) to estimate total concentrations. This highly filtered data is not ideal from a forensics perspective and can result in the data analyst missing PCB contamination from highly weathered and non-aroclor sources.

One of the key questions often asked in forensic investigations is *how many PCBs are present in the environment and where have they come from?* This presentation will provide a brief overview of known aroclor and non-aroclor sources of PCBs. It will discuss which congeners are commonly detected in the environment and will present data obtained from marine animal samples analysed by GC-qqqMS and GCxGC-ToFMS. The results show that over 150 congeners were detected in the samples, with conservative estimates indicating that approximately 5% of the total PCB concentration in some samples originated from non-aroclor sources.

CongenerR: A TOOL FOR COMPARING PCB-
CONGENER DATA WITH DIFFERENT CO-ELUTION
PATTERNS

Koshlan MAYER-BLACKWELL^{*1}, Jeffrey S. PARKER¹

¹ Pacific Groundwater Group, 2377 Eastlake Ave E. Seattle, WA
98102

* Presenting Author

Polychlorinated biphenyls (PCBs) are a class of 209 chemicals that are of concern due to their environmental persistence, bioaccumulation, and carcinogenic effects. Inconsistencies in PCB congener datasets can originate from non-uniformity in laboratory protocols for EPA Method 1668. For example, comparing data generated using DB-5 or SPB-octyl chromatography columns is confounded by different congener co-elution patterns (Rodenberg et al. 2015). These methodological variations can be overlooked by regulators and consultants charged with generating PCB congener datasets. Under ideal circumstances, only one type of GC column should be used to evaluate PCB congeners within a given study area;

however, cross-study comparisons and the analysis of historical datasets sometimes require using data generated with different GC columns. To interpret congener data generated using different GC columns, we are developing a software tool for rapid comparison and visualization of PCB congener results generated from different co-elution patterns. The tool is written for use in the open-source R statistical environment. We evaluate its use given a number of simulated weathered and raw Aroclor mixtures and assess under what circumstances inconsistently generated Method 1668 data may be useful for reaching qualitative forensic conclusions.

A PCDD/F FINGERPRINT STUDY USING THE 190
NONTOXIC CONGENERS: FIRST RESULTS

Carlo Monti^{1*}, Nicholas Rose², and Tim Negley³

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² TIG Environmental, 112 W 34th Street, 18th fl., New York, NY

³ TIG Environmental, 443 North Franklin St, Suite 220, Syracuse, NY

* Presenting Author

A study has been carried out on the fingerprint of the 190 nontoxic PCDD/F congeners. The scope of the study is the definition of the congeners that identify the 190 nontoxic PCDD/F fingerprint in some environmental media in an industrial/agricultural area in Southern Italy (Taranto, Puglia, Southern Italy).

Samples of soils, pine litter and pasture grass were sampled in the urban area of the city of Taranto and in the surrounding agricultural area. Ten sites were identified and sampled. Samples were analyzed for the 190 nontoxic PCDD/F by Analytical Perspectives (now SGS Environmental Services) using high-resolution gas chromatography-high-resolution mass spectrometry (HRGC-HRMS).

Congeners with more than 50% of non-detected concentrations were excluded from the analysis. Therefore, 66 congeners were retained for the fingerprint analysis. Of these, nine are four substituted dioxins (4D), seven are 5D, four are 6D, one is 7D, twenty-three are 4F, eleven are 5F, nine are 6F and two are 7F. A final dataset was defined of 66 congeners and 28 samples (10 samples of soils, 8 of pasture grass and 10 of pine litter).

All statistical analyses were performed using the multivariate software package Unscrambler 10.1 (Camo Software, 2015). Non-detected results in the final dataset were substituted with values estimated by multivariate linear regression and a PCA was conducted on this final dataset. Results indicated that five congeners explain 95% of the total sample variance. The congeners were 123468D (6D), 1234679D (7D), 1347F (4Fa), 2367/3467F (4Fb) and 124678/134678F (6F).

In pine litter samples, 4Fa and 4Fb were the dominant congeners (20-36% and 23-36% respectively). In soil samples, the dominant congeners were the two 6D, 7D, and 6F (15-27%, 18-42% and 18-31%, respectively). A sample of soil taken in the urban environment was an exception and the dominant congeners were 6F and 4F. Pasture grass composition was highly variable.

Comparing the composition of the soil, litter and pine litter samples in the same sampling station, the pine litter and pasture grass samples show an enrichment in percentage in the two 4F congeners. In pine needle samples the relative percentage of the other congeners remains constant. This difference between the soil, the pine litter, and the pasture grass samples seems to indicate a different source in recent years or a different degradation time of 4F as compared to the other congeners.

A MATLAB TOOL FOR VISUAL GOODNESS-OF-FIT EVALUATION IN MULTIVARIATE ANALYSIS OF PCB AND PCDD/F CONGENER DATA

Glenn JOHNSON*¹

¹University of Utah, Salt Lake City, Utah, U.S.A

*Presenting Author

In publications going back to 2000 (Johnson, et al., 2000, I have advocated that, in multivariate analysis of environmental chemical data, one should evaluate goodness-of-fit on a variable-by-variable basis (i.e. congener-by-congener). Specifically, for each number of principal components or sources considered, one plots an array of CD-scatter-plots. This is a graphical extension of Miesch's (1976) coefficients of determination (CD table) for each chemical in a PCA or "factor analysis."

Where n is the number of congeners in a PCA or receptor model, a CD scatter-plot array is a series of n scatter plots, with each corresponding to a different congener. The measured values of all samples in the model are plotted on the x-axis, against the back-calculated values for a given number of principal components or end-members on the y-axis (Figure 1). In contrast to single scalar goodness-of-fit indices (e.g. percent-variance accounted-for in PCA) a CD scatter-plot array allows one to evaluate goodness-of-fit for each congener separately. It also facilitates identification of outliers, which help determine of the correct number of principal components or sources to retain for a PCA or mixing model.

The use of CD scatter-plots is most closely associated with polytopic vector analysis (PVA) because it was developed by practitioners of methods within that academic lineage (mathematical geology). It is however, applicable to PCA or any receptor model method. In this paper, I present a software tool (a Matlab utility) that allows one to plot CD scatter-plot arrays using output typically provided in reports/papers that use methods other than PVA. Example applications will be shown using reported results or the reproduction of a PCA, PMF, or NMF solution, as reported in literature or 3rd party consultant reports.

References

- Johnson, et al., 2000. Resolving polychlorinated biphenyl source fingerprints in suspended particulate matter of San Francisco Bay. *ES&T*, 34, 552-559.
- Johnson, G.W., Ehrlich, R., Full, W., and Ramos, S. (2015). Chapter 18: Principal components analysis and receptor models in environmental forensics. In: *An Introduction to Environmental Forensics*. 3rd Edition. Morrison & Murphy, eds. Elsevier. 609-653.
- Miesch, A.T., 1976. Q-mode factor analysis of geochemical and petrologic data matrices with constant row sums. USGS Prof. Paper 574g.

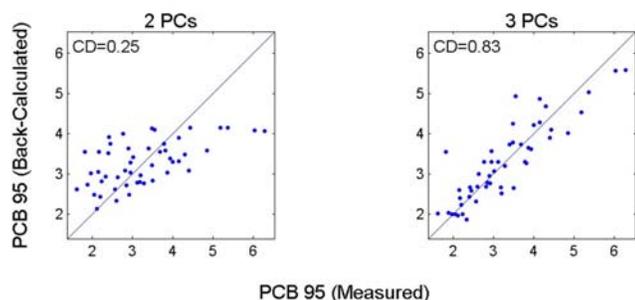


Figure 1. CD Scatter plots for a single congener (PCB-95) for $n=2$ and $n=3$ principal components, from an analysis of a 50 sample, 56 congener data set.

EAST CONFERENCE ROOM: SESSION 10: METALS

EVALUATING THE SOURCE(S) OF METALS AND METALLOIDS IN RESERVOIR SEDIMENTS – GEOGENIC OR ANTHROPOGENIC?

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*Presenting Author

Successfully planning and executing environmental investigations of land and water bodies associated with industrial sites potentially impacted by metals and metalloids are challenging for many reasons, with perhaps the greatest challenge determining whether the metals and metalloids are from natural processes (geogenic), from recent or historic industrial operations (anthropogenic), or from other human activities. Several geochemical methods and tools are available that support evaluating whether metals and metalloids are geogenic or anthropogenic, and taken together can support differentiating multiple anthropogenic sources. We used these techniques to evaluate sediments at a large freshwater reservoir immediately adjacent to a former industrial facility in the mountains of southern California.

The geochemical methods used for the reservoir case study included whole-rock analysis using x-ray fluorescence to yield elemental concentrations; and optical petrography, powder x-ray diffraction, and electron microprobe to determine what minerals are present and the distribution of elements in minerals.

A case study will be presented for which many of these techniques were successfully utilized to demonstrate, using multiple lines of evidence, that metals and metalloids present in reservoir sediments were primarily geogenic and unrelated to recent industrial operations at the adjacent industrial site. However, some anthropogenic metals were identified. Critical features identified in the case study included (1) documenting locally significant metal sulfide, metal arsenide and metal oxide minerals of a form and composition typical of natural hydrothermal and magmatic mineralization; (2) documenting the presence of a suite of elements characteristic of hydrothermal mineralization; (3) defining present-day geochemical conditions and consequent stability of minerals in the sediment and at the sediment-water interface; (4) documenting mineral textures that, with the above features, provide information on the conditions of mineral formation, including examples of mineral origin by hydrothermal, in-situ (reservoir bottom but not site-impacted), and anthropogenic processes.

APPLICATION OF PINE NEEDLES AS BIOINDICATORS OF TRACE METALS IN URBAN AIR

Kevin Hayes,¹ Gwen O'Sullivan¹, & Alexander Ursino¹

¹ Mount Royal University, Calgary, Canada

*Presenting Author

Air pollution has been recognized as a problem throughout history. The concentration of people in urban environments and the associated increase in traffic emissions has led to a decrease in air quality in the urban environment. Air pollution research today is examining the linkage between air pollutants and health implications and refining our understanding of risk from a general population scale to a community level. Our ability to study a finer scale has been limited by our monitoring programs. This study

looks at the collection and analysis of foliar samples (proxy indicators of air quality) to examine variation in urban air quality at the community level and explore the linkage, if any, with socioeconomic status of a community.

Biomonitoring of trees, in particular needles, has commonly been used to examine the impacts of air quality on forest ecosystems and more recently urban environments. We will present the findings from a study in which foliar samples were collected at the community level within an urban setting. The concentration of trace metals were determined using ICP-MS. Multivariate statistical analysis, including principal component analysis, was completed to determine trends and relationships within the data. The presentation will highlight the potential, and limitations, of biomonitoring using pine needles, to assist with our understandings of baseline environmental conditions and the environmental impacts of urban air pollution.

RECORD OF LEAD POLLUTION IN GREAT SALT LAKE SEDIMENTS

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* Presenting Author

Mining, industrial and agricultural activities, fossil fuel burning, and building infrastructure are responsible for the abrupt increase in lead introduced to the biosphere globally during the past centuries. Mining activities in Utah developed quickly into large-scale operations after the first transcontinental railroad was completed in 1869 and remained the main commercial activity in the region for the next decades. Early mining districts that were either part of the endorheic Great Salt Lake (GSL) watershed, draining through the Jordan River, or part of northern Utah's main airshed, extensively added to the lead load in GSL sediments.

Using lead enrichment factors and isotopic ratios from a GSL core obtained in Farmington Bay we show how the different lead sources played out during the last centuries. Enrichment factors tripled in 200 years since late 17th century levels, with the main change emerging during the 19th century. However, it was between 1875 and 1920 when the major pollution occurred, with an additional increase by a factor of 5 and reaching levels of almost 16. A slow decline reaching a value of 14 then followed until the late 1950s, when a moderate increase ensued with a local maximum around the 1970s. On the other hand lead isotopic ratios changed continuously towards less radiogenic values with the largest change happening during the 18th century when the amount of lead doubled. This initial drift moved along the same general direction until the 1920s, when an abrupt change towards more radiogenic ²⁰⁶Pb/²⁰⁴Pb started. Finally, a distinct trend starting in the 1960s showed a local maximum in ²⁰⁶Pb/²⁰⁴Pb and ²⁰⁸Pb/²⁰⁴Pb during the 1980s, suggesting a moderate contribution from leaded gasoline in the region. The combination of enrichment factors and isotopic ratios measured in sediments was valuable to parse the contamination history as well as to assess the relative importance of the main lead sources impacting the Great Salt Lake basin. Our data suggests that lead derived from early mining activities in Northern Utah remains by far the principal addition of lead in this region.

IMPLEMENTATION OF CIRCULAR ECONOMY IN TREATMENT OF LANDFILL LEACHATE

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* Presenting Author

With landfills becoming overloaded or limited, there are constant efforts in place to minimize waste going to landfills. In order to move from a linear metabolism in solid waste handling where useful resources are wasted to a circular metabolism where useful resources are recovered, the inherent economic and environmental benefits and, the risks have to be identified. There is a growing need to recover useful products such as nutrients from waste and recycle those back to soil system. This is circular economy. But the inherent risks associated with these approaches should be considered. There is a strong need to consider socio-economic incentives and risks associated with public health in the overall approach of circular economy. Therefore, the concept of resource recovery in landfill operations under economic and risk framework has been emphasized recently. Although, this changing paradigm of waste processing (i.e circular economy) has been well implemented in many municipal wastewater treatment facilities, its application in solid waste area has been very limited. One major challenge which preclude the application of source separation of municipal solid waste and its further use is people's perception. The appropriate technologies, protocols and government policies which ensure economic benefits and reduced risks should also be identified. The fate of contaminants need to be evaluated of emerging concerns during processes aimed at recovering useful resources out of organic waste. Furthermore, people's perception needs to be incorporated into technology development related to the processing of different types of source separated food wastes. Then, the results generated through lab and/or pilot scale testing need to be disseminated back to the people for better decision making and improved public perception about solid waste handling. People's perception about resource recovery from landfill leachate and the fate of pharmaceuticals and heavy metals during resource recovery processes will be studied in this research project. The results generated will be fed to a life cycle and economic analysis model. This research plan is built upon the present ongoing research on nitrogen and phosphorus recovery from landfill leachate followed by the treatment of leachate using innovative granular activated sludge process.



TUESDAY, JUNE 26, 2018
15:20 – 17:00

**SOUTH CONFERENCE ROOM:
SESSION 11: AIR POLLUTION**

**NO_x EMISSIONS FROM SWITCH YARD
LOCOMOTIVES IDENTIFIED WITH A LIGHT-RAIL
PUBLIC TRANSIT PLATFORM**

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* Presenting Author

The locomotive industry plays an important role in the transport of people and products nationwide. Within locomotive rail yards, switch yard locomotives (“switchers”) are used to move freight trains around to facilitate the loading and unloading of cargo. Switchers have large diesel engines that are built to last a long time, but that also means that older diesel engines currently in operation lack modern pollution control technologies. Along the Wasatch Front the switchers are primarily older models that operate within Tier 0 or 0+ EPA emission standards that have high NO_x emissions.

The TRAX light-rail based air quality measurement platform measures a suite of air pollutants and greenhouse gases (CO₂, CH₄, O₃, PM_{2.5}) and from June 2016-June 2017 the project was loaned a NO₂ analyzer to investigate the spatial patterns of NO₂ across the metropolitan area. The TRAX Green and Red lines travel adjacent to the Union Pacific rail yard in the central Salt Lake Valley and were thus fortuitously able to monitor emissions in this area. Averaged over time we observed high NO₂ concentrations, most likely due to emissions from switcher rail cars. Observations of co-located O₃ depletions due to titration provide further support for the measurements. Finally, we were able to isolate the contributions from the rail yard and the nearby I-15/I-80 interstate interchange by pairing NO₂ and CO₂ measurements.

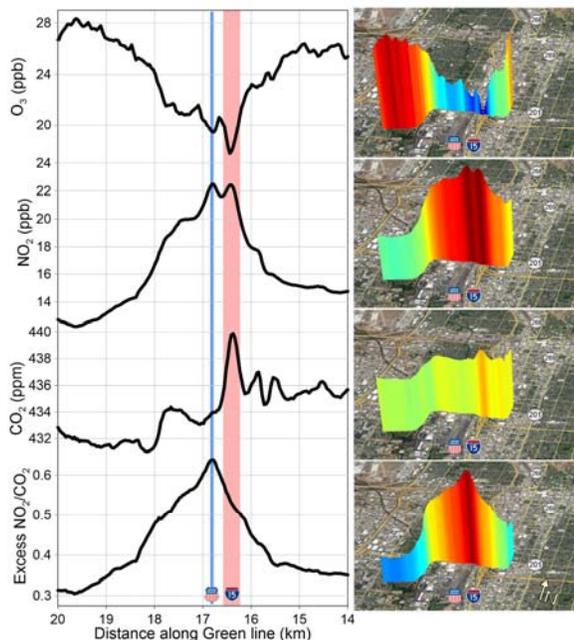


Figure 1. Relationships between species illustrating sources of NO₂ and CO₂ along a subsection of the Green TRAX line. The location of the Union Pacific rail yard and I-15 interstate highway are indicated with a blue line and red shading respectively in the left panel and with icons in both the left and right panels.

**TOWARDS IMPROVED BIOAEROSOL SOURCE
APPORTIONMENT AND MODELLING
ASSESSMENTS**

Ben WILLIAMS¹, Enda HAYES¹, Zaheer NASIR², Catherine ROLPH³, Simon JACKSON⁴, Shagun KHERA⁴, Alan BENNETT⁵, Toni GLADDING³, Gillian DREW², and Sean TYRREL²

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*Presenting Author

Bioaerosols, comprised of bacteria, fungi and viruses are ubiquitous in ambient air. Known to adversely affect human health, the impact of bioaerosols on a population often manifests as outbreaks of illnesses such as Legionnaires Disease and Q fever, although the concentrations and environmental conditions in which these impacts occur are not well understood. Bioaerosol concentrations vary, but a number of industrialised human activities such as waste and water treatment, intensive agriculture and open windrow composting facilitate the generation of bioaerosol concentrations many times above natural background levels. Bioaerosol modelling is currently undertaken using existing, proprietary models such as ADMS and AERMOD. The modelling of bioaerosols from composting facilities typically relies on proxy pollutant parameters derived from a small number of studies. Bioaerosol sampling is currently undertaken according to existing regulatory frameworks, in which the collection of bioaerosols and not the assessment of long-term trends, is of most importance. As a consequence, sampling devices are often moved around site according to changing wind direction and sampling intervals are invariably short-term. Consequently, the use of short term data gathering strategies in which monitors are moved frequently with wind direction and are not deployed during rainy days, fail to provide a robust reliable and repeatable dataset by which to validate any modelling or to assess its performance. Despite this, new sampling methods such as the Spectral Intensity Bioaerosol Sensor (SIBS) provides an opportunity to address several gaps in bioaerosol model validation and assess temporal variations. This contribution sets out the current weaknesses in bioaerosol characterisation and monitoring from the perspective of robust modelling requirements. It also sets out the means by which bioaerosol monitoring strategies can be designed to address the weaknesses in current bioaerosol model validation by considering location, duration and resolution of monitoring.

Keywords: bioaerosols, model validation, dispersion modelling, monitoring

**HOUSEHOLD INDOOR PARTICULATE MATTER
MEASUREMENT USING A NETWORK OF LOW-COST
SENSORS**

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* Presenting Author

The World Health Organization (WHO) estimates that 4.3 million people die annually from household air pollutant exposure, making indoor air quality a serious concern. Particulate matter (PM_{2.5}) of diameter 2.5µm or smaller is of particular concern

because it can penetrate into the lungs and cause serious health effects. Indoor levels of PM are significant contributors to an individual's daily exposure, and sources of indoor PM include cooking, combustion activities like burning candles or heating/cooking with solid fuel, and cleaning. Numerous studies of indoor PM measurement have employed passive air sampling or gravimetric methods. These samples are time-consuming to collect and analyze, and do not capture temporal variation. Research-grade instruments can provide accurate and rapid measurements of PM_{2.5} concentrations, but the cost of such instruments can be high, limiting the ability to place a network of sensors in a home. The objective of this study was to (1) deploy a network of two types of PM sensors (i.e., research grade instruments and low-cost sensors) in a home environment and evaluate their performance, (2) characterize activities and conditions that affect PM concentrations, and (3) identify how these activities affect different rooms in a home. The wireless sensor network included low-cost PM sensors, a gateway, and a database for storing data. The low-cost sensors used in this study were the commercially available Dylos DC1100 Pro (Utah Modified Dylos Sensor-UMDS) and the Plantower PMS sensor (Utah AirU) built at the University of Utah. These are compared to two research-grade instruments - the GRIMM and DustTrak. The study was conducted in two households in Salt Lake City, during summer and winter. The study identified activities, like spraying of aerosols and frying food, that caused PM levels to increase by factors of 2 to 4, and these elevated levels remained for several hours. Humidity also affected the PM measurements. Finally, this study identified how elevated outdoor PM levels caused by a cold air pool led to an increase in indoor PM levels over time.

RIGOROUS USE OF A CONCEPTUAL SITE MODEL TO GUIDE DEVELOPMENT OF MULTIPLE LINES OF EVIDENCE AT VAPOR INTRUSION SITES

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* Presenting Author

Vapor intrusion has become a leading concern at sites impacted by volatile organic compounds (VOCs). However, characterization of sites with potential vapor intrusion conditions has proven to be challenging due to a number of issues including uncertainties in building characteristics, short-term (diurnal) and long-term (seasonal) variations, multiple VOC sources, limited data as well as changing regulatory directives and guidance documents. In recognition of these challenges, federal and state vapor intrusion guidance emphasizes the use of a conceptual site model (CSM) to develop multiple lines of evidence (MLEs) (e.g., USEPA, 2015; California EPA, 2011; Hawaii DOH, 2014; New Jersey DEP, 2018).

This presentation will focus on the rigorous application of an adaptive framework in which the CSM is continuously refined in response to sampling results and, in turn, is used to refine the development of MLEs. For example, in a building with multiple *potential* preferential pathways, a sampling plan can be designed to identify and rule out non-functioning preferential pathways, resulting in a refined CSM that focuses resources on functioning preferential pathways. Strengths and weaknesses of sampling approaches such as discrete and time-averaged sampling will also be discussed.

The presentation will include an illustrative case study of a vapor intrusion investigation conducted as part of a property transaction that took place in Southern California. The buyer

identified a potential vapor intrusion concern and demanded a \$4.5 million price reduction. In response, the seller asked Ramboll to identify the causes of vapor intrusion and to implement mitigation measures to address buyer concerns, thereby ensuring timely closure of the deal. Using an adaptive CSM framework and a combination of innovative sampling techniques, Ramboll achieved these objectives with the result that the deal was closed and the seller realized millions of dollars of savings.

AQandU PROJECT: EVALUATION OF A LOW-COST AIR QUALITY SENSOR NETWORK IN THE WASATCH FRONT, UNITED STATES

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* Presenting Author

Low-cost particulate matter (PM) sensors are becoming more widely available and are being increasingly deployed in ambient and workplace environments due to their low cost and ability to provide highly resolved spatial and temporal PM data. However, these inexpensive sensors have limitations and need to be characterized for the conditions of use. This study consists of four laboratory and field evaluations: 1) An aerosol chamber was designed and used to assess laboratory performance of 153 Plantower PMS 3003 sensors before deploying in the field. This chamber is capable of providing uniformly distributed particle concentrations to eight low-cost sensors and a reference instrument. 2) 50 laboratory calibrated PMS 3003 sensors were deployed in different parts of Salt Lake City, UT to increase the resolution of air quality data 3) An ambient evaluation of four PMS 1003/5003 sensors occurred over two years at two state monitoring stations located in urban residential areas in Salt Lake City, UT and included elevated PM levels caused by cold air pools, fireworks and wildfires. 4) 50 sets of two co-located Plantower PMS 5003 sensors (dual sensors) deployed in different parts of Salt Lake City, UT over a period of 3 months in the winter of 2017 to investigate the inter-device agreement of the sensors.

The results showed 1) high correlations between the reference instrument (TSI DustTrakII) and the PMS 3003 PM_{2.5} readings ($R^2 > 0.978$) in the laboratory assessment, 2) PMS 3003s are capable of tracking air quality in the neighborhood scale, 3) strong correlations between PMS 1003/5003 and FEMs ($R^2 > 0.882$) and PMS 1003/5003 also maintained high inter-sensor agreement ($R^2 > 0.975$) after one year of deployment in winters 2016 and 2017, however, one of the PMS 1003s exhibited a significant drift beginning in mid-June 2017 and continued to deteriorate through the end of the study, 4) 66% of the dual sensor linear slopes agreed within 15% of each other. It is unclear if the remaining 34% agreed with each other initially and drifted over time or if they never agreed with each other.

These results have important implications for communicating results from low-cost sensor networks. They highlight the utility of these types of sensors as a relative measure of PM as well as concerns about making direct comparisons between low-cost PM measurements and those from a federal equivalent or federal reference method.

EAST CONFERENCE ROOM: SESSION 12: EMERGING CONTAMINANTS

SOURCES AND SINKS OF PBDEs IN TREATMENT PLANT SLUDGE

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* Presenting Author

Polybrominated diphenyl ethers (PBDEs) are persistent and bioaccumulative brominated flame retardants, used in upholstered furniture, electronics, insulation materials, among others. Their production and usage as commercial mixtures (penta-, octa- and deca-BDEs) are now regulated due to environmental concerns. PBDEs can easily leach from the applied products, and reach wastewater treatment plants (WWTPs). Due to their hydrophobic character, PBDEs accumulate in WWTP sludges. While tracing back the sources of PBDEs in sludge is important to realize the main contributors, projecting forward is also of great concern since application of sludge containing PBDEs on agricultural land can impact soil quality. The aim of this study is to identify possible sources of PBDEs in WWTPs in Turkey, compare them with literature, and discuss potential implications on land application of biosolids.

Dewatered sludge samples were collected from four WWTPs (two urban and two industrial WWTPs) located in four different geographical regions of Turkey. Chemical mass balance (CMB) model was used to identify possible sources of PBDEs in sludge. Deca-BDE was found to be the main contributor in three WWTPs. However, a background air PBDE profile was the main source for one of the industrial WWTPs (Fig. 1). To compare with the world data, CMB is also applied to sludge PBDE profiles from the literature. Studies on land application of sludge showed that PBDEs accumulate on applied soil, have one to four years of residence time in soil after single application, and could impact the groundwater and tile drainage.

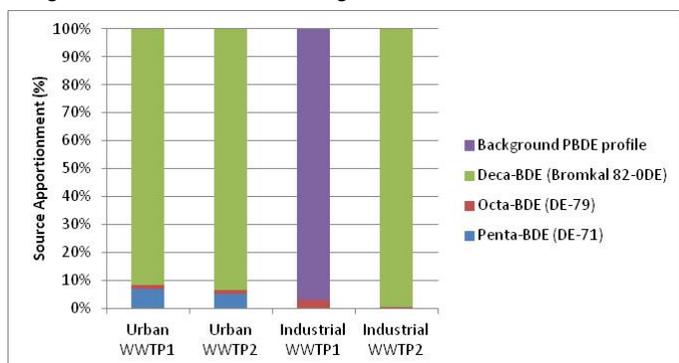


Fig.1 Source apportionment of WWTP sludge PBDEs from Turkey.

AN INVESTIGATION OF EMERGING CONTAMINANTS IN WASTEWATER: CHARACTERIZATION AND IDENTIFICATION OF BENZOTRIAZOLE DERIVATIVES BY GCXGC-TOFMS.

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Effluent waters from Wastewater Treatment Plants (WWTPs) are thought to be the main sources for contaminants of emerging concern (CECs) in the environment. CECs, including pharmaceuticals, personal care products and endocrine disrupting compounds, are present in post-treatment effluent waters due to inefficient removal at the WWTP. The Penn State WWTP utilizes tertiary treatment methods, chlorine disinfection and irrigation of crop land with effluent water, to further remove the CECs before reaching the groundwater. In this study, pretreatment influent, post-treatment effluent, spray field irrigation effluent and groundwater samples were analyzed for CECs using Comprehensive Two Dimensional Gas Chromatography with Time of Flight Mass Spectrometry (GCxGC-TOFMS). This method allowed for efficient separation of the complex water samples revealing a variety of CECs. By far the most prevalent were those of the benzotriazole compound class, utilized for their anti-corrosion properties. These compounds were not removed in the WWTP and chlorinated byproducts were formed in the tertiary treatment step. This finding led to further study including synthesis and identification of the chlorinated compounds, for which commercial standards do not exist. To the author's knowledge, this is the first study to find and attempt to identify individual chloromethyl benzotriazoles in wastewater.

MICROBIAL BINDING OF PERFLUOROALKYL SUBSTANCES (PFASs)

Ingrid ERICSON JOGSTEN*¹, Marios STYLIANO², Karolina MAJDAK¹, Petra STÄHL², Per-Erik OLSSON², and Jana JASS²

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* Presenting Author

Per- and polyfluorinated alkyl substances (PFASs) are environmental pollutants of global concern due to their persistence and widespread occurrence in humans, wildlife and the environment. These compounds have been extensively used in various commercial and industrial applications since the mid-1900. In 2009, perfluorooctane sulfonic acid (PFOS) was added to the Stockholm convention to protect humans and wildlife from harmful effects. In Sweden, severe PFAS contamination in drinking water has resulted in elevated blood PFAS concentrations in residents living in contaminated areas.

The present study evaluated microbial binding of PFASs was tested. The binding capacity was assessed in both live and dead *Escherichia coli* for various PFOS concentrations. The binding capacity of dead cells was higher (286-3324 µg/g of bacterial pellet) compared to live *E. coli* cells, showing a 5 – 7 fold lower binding capacity (38-675 µg/g of bacterial pellet). For PFOS, the

affinity of branched isomers was similar to that of linear compounds. Furthermore, other species of bacteria were tested for binding capacity of various mixtures of PFASs from both technical products and contaminated environmental waters, including *Pseudomonas nitroreducens* and *Acidovorax delafieldii*. After treatment, bacteria pellets were extracted and analyzed using liquid chromatography tandem mass spectrometry (LC-MS/MS). Preliminary results indicate preferential binding for PFOS, the contaminant present in the highest concentration in both contaminated environmental water and spiked water of the sum of eleven PFASs recommended for analysis by the Swedish Food agency.

This study gives increased knowledge of microbial binding of perfluoroalkyl substances giving insight on PFAS transport in the environment and at different trophic levels. The phenomenon of microbial binding of PFASs could also be used to establish a more cost effective remediation of PFAS contaminated waters. Further, it could lead to increased understanding of toxicological effects of PFASs related to the gut microbiota.

THE EFFECTS OF DILUTION ON BIODEGRADATION OF PHARMACEUTICALS AND METAGENOMICS ANALYSIS: IMPLICATION FOR ENVIRONMENTAL RISK ASSESSMENT

Simone Bagnis^{*1}, Mark Fitzsimons¹, Jason Snape^{2,3}, Alan Tappin¹, Pereira, G. V.¹, Sean Comber¹

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The increasing consumption and production of active pharmaceutical ingredients (APIs) in low and low-middle income countries (LLMICs) is of a growing environmental concern owing to potential ecotoxicological effects. This is related to the practice of direct discharge of untreated wastewater (DUW) into receiving waters, which creates a heavily polluted area, named the "impact zone". Little is known about the environmental fate of APIs in this area. Nevertheless, a few available measured environmental concentrations (MECs) of LLMICs show higher concentrations than for high-income countries with developed wastewater treatment infrastructures. Globally, the MECs of APIs in the "impact zone" are often above 0.01 µg L⁻¹, which, would be sufficient to trigger the environmental fate refinement of the environmental risk assessment (ERA). In the ERA PEC calculation, a dilution factor (DF) of 10 is recommended, but in at least 53 countries worldwide, the local predicted DF median observations show a lower value. There is no information available in the literature about the effects of low dilutions on the natural attenuation of APIs and in the specific case of DUW. The effects of APIs on the microbial populations at low dilution, combined with possible mixture effects is also absent, necessitating the evaluation of endpoints for the impact zone ERA. This information is pivotal for the development of an impact zone ERA approach, and we are providing novel science to further research within this field.

For instance, nevirapine shows persistency over the experimental period taking account of dilution. Acebutolol and diclofenac show a decrease in concentration of up to 90% as a consequence of dilution and/or biodegradation. Biodegradation rates appear to decrease with increasing dilution. The biodegradation of APIs in the undiluted samples shows a trend consistent with previous reported studies. Also, amitriptyline

shows persistency, though with sorption accounting for 70% of the removal from the aqueous phase.

In conclusion, the different degrees of dilution of untreated wastewater in the receiving freshwater causes variations of persistency of some APIs, whilst does not affect the persistency of highly recalcitrant compounds

IDENTIFICATION AND QUANTIFICATION OF TRACE LEVEL VOCs IN HIGHLY CONTAMINATED AIR SAMPLES

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* Presenting Author

A novel solution was developed to measure trace concentrations of selected VOCs in high concentration air matrices, utilizing conventional TO-15 canister sample collection and a standard TO-15 air concentrator. To remove interfering peaks and isolate targeted VOCs, a custom multidimensional gas chromatographic system was utilized. Compound detection was achieved using a Time-of-Flight mass spectrometer (TOF-MS) which provided improved sensitivity and selectivity as compared to a conventional quadrupole mass spectrometer. The developed method has been successfully applied to a number of challenging projects including the measurement of Ethylene Dibromide, Ethylene Dichloride, and Naphthalene at pptv concentrations in soil gas samples containing percent level total petroleum hydrocarbons.



Waters
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WEDNESDAY, JUNE 27, 2018

10:50 – 12:30

**SOUTH CONFERENCE ROOM:
SESSION 13: FORENSICS IN LITIGATION**

**CENTREDALE MANOR SUPERFUND SITE – A
LITIGATION CASE HISTORY**

Graham Ansell^{*1}, Patrick Gwinn², Russell Keenan², William Locke³

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History: In the world of CERCLA liability, the Centredale Manor Restoration Project Superfund Site provides a somewhat unique case history. Rarely, has a notified Potentially Responsible Party (PRP) argued in Court against the Agency and U.S. Department of Justice, and in some instances, received a favorable adjudication. The Centredale Manor Superfund Site is located in USEPA Region 1 and has been on the National Priorities List since 1999; primarily, for 2,3,7,8-TCDD and PCBs, but also includes PAHs, SVOCs, and 40+ other chemicals that are present at concentrations exceeding clean up levels. The litigation for this case started in 2003 with an insurance coverage case. The litigation proceeded from there and expanded into CERCLA litigation against New England Container Corporation and, eventually, bringing in the U.S. Department of Defense, USEPA, and U.S. Department of Justice. The US District Court split this CERCLA case into three “phases”, and in this presentation I will discuss on Phase I – liability and divisibility, and Phase II – costs and remedy. Phase III will be touched upon, albeit briefly, as this part of the case is currently on-going.

Conclusory Remarks: I have worked on the Centredale Manor Superfund Site for nearly 12 years; first as in-house consulting expert for two law firms, and now as consulting expert with Integral Consulting Inc. In this presentation, I hope to offer new perspective of this case from behind the scenes, on a variety of topics, including; hiring experts, litigation strategy, and, eventually, achieving a favorable adjudication in Phase II.

**THE PEER REVIEWED LITERATURE AND THE
LITIGATION PROCESS**

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The published peer reviewed literature is the pedigree of science as it documents the advancement of science through the centuries. Scientists view publishing as a requirement, the established method of advancing can communicating new ideas or developments in their field to like-minded scientists. Manuscripts are written and sent to the managing journal editor for subsequent review and discussion before a finished paper is released to the entire scientific community. During the peer review process, manuscript reviewers and journal editors read,

question, validate, discuss and evaluate the work for the expressed purpose of advancing scientific inquiry as their predecessors have done before them for decades or centuries. Only after what is no less than a required exhaustive review process does the manuscript become published and available to the entire scientific community.

An environmental forensic scientist, when qualifying as a testifying expert in the litigation process, draws on a body of technical information that is available to all. Such information includes what is available in the peer-reviewed literature as well as what might be developed during the course of the litigation process. Having technical information available in the literature, however, is not enough for the legal setting. With the judges acting as the gatekeepers to the admission of technical information to the proceedings, there are requirements that are placed upon the testifying expert as well as their use of the peer-reviewed literature. This paper will discuss the relationship between the peer reviewed literature and the expert working with the litigation process from the perspective of the obligations both incurred and engendered.

**NO SMOKING GUN? ENVIRONMENTAL FORENSIC
METHODS TO STILL BUILD A WINNING CASE**

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Historical research plays a critical role in environmental forensic investigations in trying to answer the questions related to a contaminant release of Who?, What?, Where? and When? Development of the historical site history and past operations is a critical step in trying to determine the nature and timing of a contaminant release and identifying the potentially responsible parties (PRPs). Seeking out evidence to prove a certain PRP contributed to the contamination is oftentimes a laborious task, consisting of hundreds of hours of in-depth research and analysis. Few times, do you find the “smoking gun” piece of evidence, directly linking a party to the contribution. However, with careful due diligence and a comprehensive analysis, making that connection can prove successful. By combining various lines of evidence with historical information such as historical aerial photographs, Sanborn Fire Insurance Maps, World War II and military records, old trade publications and newspaper archives, building permits and disposal records, just to name a few, a comprehensive site history with multiple strong lines of evidence can be established to help reconstruct the contaminant release and help win the case.

This presentation will review the various sources of information that can be used to build a comprehensive case using multiple lines of evidence in order to identify the PRPs and their connection to the contaminant release. Examples of historical resources will be presented, how they can be accessed, and the tips and tricks of the trade in finding the documents necessary to build the case. Each research case is different, and utilizing these sources of historical information may or may not provide the information needed. Therefore, developing a pragmatic research program and outlining the objectives is essential in identifying what information needs to be obtained. Three real world case studies will also be presented, providing examples of how these historical sources of information helped meet the objective of each case, but they will also reveal the often disparate nature of each case in terms of the variability in available historical information. The three case studies will

include a historical pipeline release in Los Angeles, identification of historical PRPs in relation to a solvent groundwater plume in a major metropolitan area, and arsenic and metals at a school site.

ENVIRONMENTAL REMEDIATION STUDY DESIGN: THINKING THROUGH TO A FORENSICS / LITIGATION END

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Rarely is the forensics investigator standing where or when anthropogenic release(s) occur. Indeed overwhelming experience has shown that it is much more likely that forensics assessments are requested well after site remediation. Rarely is there an opportunity for input before site engineering work begins for such things as overall study design, target matrices, sample collection, analytical methods selection, or data collection/archiving procedures. Much of this issue is inherent in regulatory requirements. However, much more of this issue has to do with the inherent goals of environmental remediation itself.

Environmental site remediation work is cleanup. Work is focused only on removing known contamination, with the end goal of achieving a regulatory site closure ruling. If leaking underground storage tanks (USTs) are the source of contamination, their isolation, cleanout, and eventual removal from the site are major priorities that quickly occur. For example, in singularly focusing on UST removal, valuable forensic evidence, i.e., detailed product composition data, can be lost quickly with no opportunity for recovery. As site work proceeds, approaches used for tracking contamination to isolate and remove contamination are regulatory based. As such, additional forensic details necessary to characterize soils, water or separate phase liquid can be lost and, once the contaminated matrices are gone, again there is no opportunity for recovery.

Analytical methods employed in remediation of anthropogenic releases can vary greatly. Usually regulatory limit is the issue and once the limit in soil or water is achieved, data collection work stops. Some level of forensic information can be gathered from regulatory methods used; however, much more can be gained by applying data intensive forensic analytical methods. How resulting data are assembled, displayed and archived matters. Analytical reports contain valuable information. All too often copies of analytical laboratory reports are at first assembled somewhere but then eventually lost. Reconstruction of the assembled data manually then has to come from summary level report tables, something replete with error opportunities. Moreover, reconstructing laboratory reports themselves becomes less and less possible over time.

To address such issues, a matrix approach is proposed to ease the transition of a regulatory based site remediation to a forensic investigation using technically valid procedures on both counts. A recently completed technical assignment for investigation of subsurface gasoline releases is reviewed to illustrate both positive and negative consequences of such efforts.



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USING THERMODYNAMICS TO IDENTIFY AN ATMOSPHERIC PCB SOURCE

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Anniston, Alabama was a site of polychlorinated biphenyl manufacturing from about 1929 to 1971. During production about 5000 metric tons of PCB production waste were dumped into a landfill in an old quarry about 500 meters to the southeast from the plant. It was suspected that PCBs measured in the air in the atmosphere in Anniston during the late 1990s were originating from this landfill. During early litigation against the manufacturer, it became apparent that one of the defendant's greatest concerns - and that it would fight - was being required to remove PCB material from this landfill. What scientific evidence can be used to identify such a landfill as a source of atmospheric PCB?

Many investigations of gas-phase atmospheric PCB show a strong relationship between concentration and air temperature, especially near PCB sources. Comparative gas phase atmospheric PCB trends during an annual temperature regime at two sites near the former PCB manufacturing plant in Anniston indicate a departure from this trend. The Mars Hill sampling site, located closest to the plant and landfills, shows an annual average Σ PCB concentration of 27 ng m⁻³ (ranging from 8.7 – 82 ng m⁻³) three times the average at Carter, 1.5 km away (9 ng m⁻³, ranging from 1.1-39). However, total PCB and congener concentrations vary more with air temperature at Carter where PCB are evaporating from surfaces during warmer weather. The slopes of the Clausius-Clapeyron plots of 18 of the most concentrated congeners representing dichloro- through heptachlorobiphenyl homologues are significantly higher at the Carter site. While some of the atmospheric PCB at Mars Hill was probably derived from ground surface evaporation, the source of most of it apparently is the material buried in the landfills which have different thermal properties than surface materials, and are not in equilibrium with air temperature.

Using thermodynamics via the Clausius-Clapeyron equation in this situation showed without question that PCBs were being emitted from the landfill and that those PCBs were moving off plant property, a major issue in contaminant litigation cases.



EAST CONFERENCE ROOM:

SESSION 14: EMERGING ANALYTICAL METHODS

DEVELOPING FORENSIC TOOLS TO EVALUATE THE RESULTS OF NON-TARGETED CHEMICAL ANALYSIS

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Advances in analytical methods have greatly increased the number of compounds detected in environmental matrices. While one dimensional gas chromatography mass spectroscopy (GC-MS) can measure the concentrations of 10s of compounds per sample, non-targeted two dimensional gas chromatography (GCxGC-MS) can identify 100s compounds per sample. High resolution mass spectroscopy, with or without chromatographic pre-separation, may identify 1000s of chemical formula per sample.

This presentation will describe the development of data evaluation approaches that can be used on the results of non-targeted analysis of environmental samples to translate data into information. Some are based on traditional forensic tools such as principal component and hierarchical cluster analysis while others incorporate approaches from different fields, such as the application of ecological species diversity assessment algorithms to assess sample chemodiversity. Depending on the method, they can be applied with-in Excel or through the use of statistical programs such as R or Matlab.

A case study will demonstrate the use of these methods to compare chemical mixtures associated with hydrocarbon biodegradation found in groundwater at petroleum release sites. Results from non-targeted analyses using GCxGC-MS and Orbitrap high resolution MS will be presented.

CHANGES TO POLYCHLORINATED BIPHENYL (PCB) SIGNATURES AND ENANTIOMER FRACTIONS IN DIFFERENT TISSUE TYPES

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Comprehensive multidimensional gas chromatography (GCxGC) was developed at the end of the 20th century. The technique has several advantages over single dimensional chromatography as it can significantly increase peak capacity (selectivity), increase sensitivity and reduce analysis times. Despite these advantages the technique has not been as widely used as might be expected. The excellent separation provided by GCxGC makes it ideally suited to the determination of PCBs, yet only approximately 2% of papers published on PCBs in the last decade have used the technique.

This presentation introduces a case study which highlights the applicability of GCxGC for chemical fingerprinting of PCBs in wildlife. Two sea bird carcasses (Common Guillemot – *Uria aalge*) were dissected, each providing 12 discrete samples of different tissue types and 3 samples of partially digested food. A total of one hundred and five PCBs from the 209 determined by GCxGC-ToFMS were detected in the samples. The relative proportions of individual PCBs did not vary greatly within tissue types, although the PCB profile from undigested food could be clearly distinguished. Enantiomer fractions (EFs) were determined for CB-95, CB-136 and CB-149 by GC-HRqToFMS. EFs in the partially digested food were near racemic, with high levels of enrichment for E1 CB-95 in the kidneys and liver (EF of 0.80 and 0.84 respectively). This provides some of the clearest evidence to date that fractionation takes place in the organs where metabolic biotransformation and elimination of PCBs occurs. Our findings also confirm the ability of non-lethal sampling techniques, such as collection of small (< 1 g) blood samples, to provide PCB signatures that are representative of an individual organism.

ONLINE MONITORING OF VOCs FROM WASTE EFFLUENT BY GC-FID AND GC-TOF MS

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* Presenting Author

Current spot checks are no longer satisfactory to avoid the potential for high-level contamination of rivers or estuaries from industrial waste. Governing environmental bodies can impose heavy fines on companies that routinely exceed the set limits, and even reserve the right to shut down the liable plant.

This produces a requirement for online monitoring of multiple outlet streams from the plant, before and after potential dilution points. Monitoring the river for contamination from other sources is also required to protect against false liability claims.

Here, we utilise a flow-through cell for online effluent sampling, with time-saving robotic tool change for sampling, standard addition and headspace analysis on a single, fully-automated platform. The use of GC-FID for analysis enables remote, continuous monitoring for rapid response to contamination events, while GC-TOF MS provides confirmatory analysis and identification of unknowns or compounds of emerging concern.

NUCLEAR MAGNETIC RESONANCE: AN IMPROVED SOURCE FINGERPRINTING ANALYTICAL TOOL

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Conventional analytical methods used to characterize complex non-aqueous phase liquids (NAPLs) generally rely on chromatographic separations of individual compounds. These approaches are limited because analytical standards for many NAPL constituents are not readily available, and because the dilutions required for these methods reduce the sensitivity for minor constituents. As such, a significant portion of the composition of a complex NAPL often remains uncharacterized. Nuclear magnetic resonance (NMR) spectroscopy has many potential advantages, including the ability to analyze samples without significant dilutions and the production of molecular spectra for compounds that can be used to identify unknowns.

NMR can be used to identify and quantify a broad range of compounds in a single analysis. Research has been underway to develop methods and a database of standard NMR spectra to facilitate rapid characterization of complex NAPL mixtures.

NAPL samples were collected from three sites with different overall contaminant profiles (coal tar, chlorinated/nitrated benzenes, anilines, chlorofluorocarbons, chlorinated hydrocarbons). These samples were analyzed using a variety of NMR methods, including ¹H, ¹³C, and ¹⁹F NMR, and multidimensional analysis. NMR findings were compared to the gas chromatography-mass spectroscopy (GC-MS) or gas chromatography-flame ionization detector (GC-FID) results. NMR provided a more complete and comprehensive analysis than GC-MS employing standard EPA methods. For most samples, 0% to 9% of the composition in the NAPL samples was characterized by the GC-MS methods tested here. Conversely, the NMR methods employed in this study were able to identify 70 to 99.9% of the composition of these samples. The discrepancy originates from the underreporting of the contribution of major NAPL constituents by GC-MS, likely due to the dilutions required to prepare these samples for analysis. Another advantage of NMR over GC-MS lies in the characterization of structural isomers. In general, GC-MS methods often suggest the presence of many structural isomers that are not supported by the NMR data.

IDENTIFYING AND QUANTITATING NON-TARGET ENVIRONMENTAL POLLUTANTS BY USING A ROUTINE COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY METHOD

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With over 100,000 chemicals of commerce routinely used on a daily basis, the need for multiresidue methods to prioritize the monitoring of potentially persistent, bioaccumulating and toxic contaminants is increasing. Comprehensive two-dimensional gas chromatography (GCxGC) is known to be one of the most powerful techniques for the separation of complex environmental samples, especially for the analysis of compound groups that contain congeners or homologues like polychlorinated biphenyl congeners (PCBs). The enhanced selectivity of GCxGC enables the less selective micro electron capture detector (μECD) to be an ideal tool for routine target compound analysis, and can also be used for assessing the presence of non-target contaminants. The μECD is very sensitive to halogenated compounds and is an excellent detector for quantitative analysis. In addition to targeted analysis, when “unknown” peaks are observed in the two-dimensional chromatograms, further investigation is performed by using GCxGC-time-of-flight mass spectrometry (TOFMS) to provide preliminary identification. The case study presented emphasizes that using a technique such as GCxGC-μECD used for the routine testing of environmental samples is an excellent screening approach for detecting non-targeted contaminants. Following up the initial identification by GCxGC-μECD and confirmation by GCxGC-TOFMS of the observed “unknown” peaks, quantitative and semi-quantitative approaches were applied for compound classes such as polychlorinated diphenyl ethers. As a result, mono- to nona-chlorinated diphenyl ethers were detected and quantified in core sediment and fish samples collected from Lake Ontario, Whitby Harbour, Ontario. Examples of a number of other identified compounds in complex environmental samples will also be presented.



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POSTERS

WEST CONFERENCE ROOM

CHARACTERIZATION OF COMMUNITY URBAN AIR QUALITY USING TREES AS BIOMONITORS

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Airborne pollutants, including heavy metals, are capable of travelling large distances in the form of aerosols. These contaminants can occur naturally, but are often linked to anthropogenic activity including industrial processes and the combustion of fuels. Due to increased local population, these activities are concentrated in urban areas. Plants can be used as a passive sampling mechanism to monitor this pollution. Coniferous trees, and more specifically, the tree's bark and needles, have been used successfully in the past for this purpose.

For this work, needle samples were collected from multiple urban locations in Calgary, Alberta, Canada in 2016. Additionally, needle/leaf, bark, and soil samples were collected from both coniferous and deciduous trees on Mount Royal University campus in 2017 in the same city. The needles and leaves were dried, ashed, and acid digested. The prepared needles and other sample types were subsequently analyzed utilizing Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Single and multivariate statistical methods are employed to determine the relationship between the various collection locations, the type of trees, as well as, the relationship between the leaves/needles, bark, and soil as uptake sites.

EXPOSURE DETECTION OF A VARIETY OF PHARMACEUTICALS AND PERSONAL CARE PRODUCTS IN DOMESTIC RECLAIMED WASTEWATER REUSE PRACTICES, IN NORTHERN UTAH

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Previous research has shown that some pharmaceuticals and personal care products (PPCP) are not removed from domestic wastewater by conventional treatment methods. Reuse of treated wastewater for urban or agricultural irrigation raises the concern of how those compounds can affect humans exposed to them in various ways. This USDA-NIFA funded study focuses on detection and exposure assessment of 12 PPCPs in wastewater influent; effluent; reclaimed water used for irrigation; soil, plants, fruits and vegetables (cucumber, beet, potato, squash, and onion) grown with reclaimed water; and aerosols generated in active irrigation systems in Northern Utah. Twelve PPCP compounds quantified in this study included Acetaminophen, Caffeine, Deet, Sulfamethoxazole, B-Estradiol,

Estrone, Progesterone, Gemfibrozil, Carbamazepine, Triclosan, Fluoxetine and Tris-(2-chloroethyl) Phosphate. Quantification of these compounds was done in water samples through solid phase extraction methods followed by Triple Quad LC/MS System. For plant, fruit and soil samples the same procedure was used after samples were dried, lyophilized, and passed through an ASE (Accelerated Solvent Extraction) method.

In another part of this research various methods for detection of these 12 PPCPs in aerosols from sprinkler irrigation were investigated. Various sampling methods (filters; and all glass impingers connected to portable, battery-operated MiniVol samplers) were evaluated to define optimal operating procedures for quantifying exposures to PPCPs in aerosols generated in sprinkler irrigation of reclaimed wastewater. A series of experiments were conducted using a concentrated PPCP spiked impinger solution. These tests were repeated using: 1) different impinger solutions (distilled water; and 80%:20% methanol: distilled water solution); 2) various sampling durations: 3, 6, 12 and 24 hours; and 3) using one impinger or two impingers in series. As a result, the recovery of the all PPCP compounds were tested and compared in order to define the best impinger solution, sampling duration and impinger configuration for the detection of PPCPs in aerosols generated at active irrigation sites. The potential reuse risks associated with these PPCP are discussed in this study based on these results.

METHOD OPTIMIZATION AND VALIDATION OF COMPREHENSIVE MULTIDIMENSIONAL GAS CHROMATOGRAPHY USING RESPONSE SURFACE METHODOLOGY FOR THE APPLICATION OF IGNITABLE LIQUID RESIDUE ANALYSIS

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Wildfire debris samples are complex matrices which present a very intricate mixture of compounds. Identifying ignitable liquid residue (ILR), in suspected arson debris samples can be challenging when facing the presence of unresolved complex mixtures from matrix and background. Comprehensive two-dimensional gas chromatography (GCxGC) coupled with time-of-flight mass spectrometry (TOFMS) is seen as a potential tool to transform the analysis and determination of ILR with its increased separation potential and detection limits (compared to GC-MS).

Due to more complex instrument aspects, a primary and secondary column, GCxGC method development and validation can be more challenging than traditional GC analysis. To address these challenges, this study examines the importance

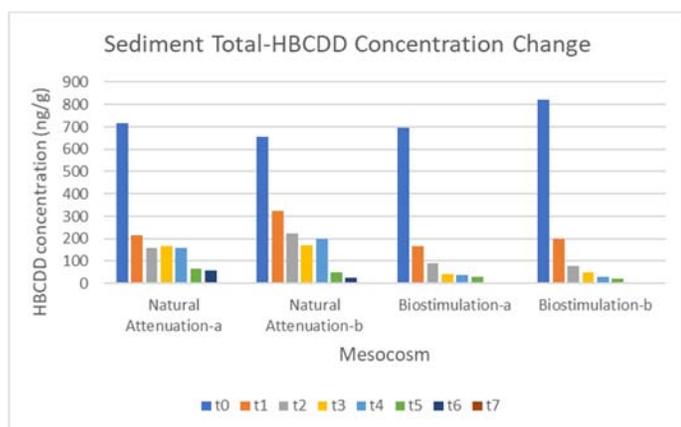
and challenges of method development including the benefits of response surface methodology. Two such designs, Doehlert and Box-Behnken, were used to examine the influence of instrument and run parameters to enhance resolution, sensitivity and selectivity for ILR compounds. Validation of enhanced methods was completed via analysis of ignitable liquid residue from wildfire scenes using peak indices as response factors.

HEXABROMOCYCLODODECANE (HBCDD) BIODEGRADATION IN ANAEROBIC SEDIMENT MESOCOSMS

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Hexabromocyclododecane (HBCDD) is a brominated flame retardant which is listed as a persistent organic pollutant (POP) and regulated by the Stockholm Convention on POPs. There are currently a very limited number of studies in the literature on HBCDD degradation, and - to the best of our knowledge - no mesocosm-scale study evaluating anaerobic biodegradation in HBCDD contaminated sediments. In this study, anaerobic biodegradation of HBCDD was investigated in two laboratory sediment mesocosms (2L) set up to simulate natural attenuation and biostimulation. In addition to HBCDD spiked sediments, natural attenuation contained only distilled water while biostimulation was prepared by adding organic medium containing electron donor (ethanol) and carbon source (sodium formate). There were also contaminant control and sterile mesocosms as control. All reactors were run in duplicate, prepared under N₂:CO₂:H₂ environment in an anaerobic glovebox (PlasLabs 818GB/Exp), incubated in the dark at 25°C. Mesocosms were operated for 49 days, sampling every 7 days. During analysis of HBCDD, GC-MS was used for total-HBCDD and LC-MSMS for evaluation of α , β , γ -HBCDD diastereoisomers. As a result, percent reduction in total-HBCDD, and α , β , γ -HBCDD as well as degradation rates were obtained for natural attenuation and biostimulation, and compared with available literature on HBCDD degradation. This study was funded by Scientific and Technological Research Council of Turkey, Project No: 115Y122.



ASSESSMENT ECOLOGICAL RISK OF HEAVY METALS IN FARMLAND: A CASE STUDY IN CHINA

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Project supported: The State Key Research & Development Program of China (2016YF0503604)

Artisanal Pb-Zn smelting activities, which had been widely applied in Bijie City, Guizhou Province, south-western of China, can pollute surrounding farmlands. For several decades since 1980s, large quantities of heavy metals have been released into the environment without proper treatment, which seriously threat the ecological environment and human health.

The goal of this study was to evaluate ecological risks of heavy metals in farmlands by applying Hakanson risk evaluation method. Topsoil samples in farmlands were collected and measured the content of eleven kinds of heavy metals, Arsenic (As), mercury (Hg), copper (Cu), lead (Pb), zinc (Zn) and etc., by using inductively coupled plasma mass spectrometry (ICP-MS). Using the single factor ecological risk index, the soil in this study cases showed a strong risk level of Cd, Pb, Zn and As. The ecological risk of heavy metals in farmland soils is in the order of Cd>Pb>As>Zn >Cu>Ti>Co>Cr>V>Mn>Ni. It could be concluded that the ecological risk of the farmlands was comparatively notable.

Keywords: heavy metals, ecological risk, farmland, China

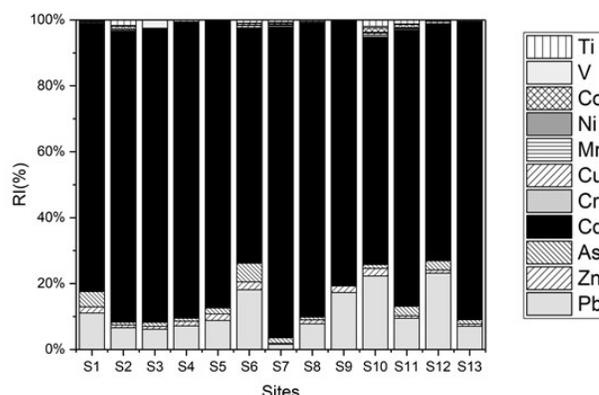


Fig. 1 Percentage of ecological risk index (RI%) of heavy metals in farmland soil

DUAL-CHANNEL GC×GC-FID FOR ROUTINE TPH ANALYSES

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The determination of aliphatic/aromatic compounds when performing Total Petroleum Hydrocarbon (TPH) analysis is typically a lengthy process – with solid phase extraction (SPE) to separate aliphatics into hexane and aromatics into dichloromethane, prior to two separate GC analyses per sample.

The enhanced separation of comprehensive two-dimensional chromatography (GC×GC) negates the requirement for

laborious sample fractionation, saving a significant amount of extraction and processing time, while also reducing consumable costs. Instead of two separate analyses, the traditional 'boiling point' separation is maintained in the first dimension while the aliphatic and aromatic compounds are separated in the second dimension.

Fast and confident group-type quantitation is then performed, using simple data processing tools. Stencils are applied to group peaks into chemical classes (e.g. C₈-C₁₀, C₁₀-C₁₄ etc) based on their elution region. The use of flow rather than thermal modulation, ensures excellent retention time repeatability across large sample batches, enabling automated data processing to be performed with minimal operator intervention.

Furthermore, here we demonstrate a dual-channel configuration, doubling the sample throughput per instrument - increasing productivity, reducing bench space and lowering installation costs, all while meeting the criteria set out in standard methods (e.g. TPH Criteria Working Group and Massachusetts Department of Environmental Protection).

RECENT TRENDS IN ANALYTICAL METHOD FOR THE DETERMINATION OF PCBs

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Polychlorinated biphenyls have been monitored in the environment for over 50 years. Early methods focused on gas chromatography electron capture detection (GC-ECD), however over time techniques including comprehensive two-dimensional GC, high resolution and tandem mass spectrometry have been developed. Analytical methods have shifted from determining Aroclor equivalent concentrations to trying to separate and

quantify specific PCB congeners. This research presents an overview of current state of analytical methods and identifies recent trends over the last decade.

In order to construct both a systematic and thorough search of the literature, the strict search term "*PCB* AND *Polychlorinated biphenyl* AND *environment* AND *Analysis*" was employed using the Web of Science database. Following this, abstracts and papers were read to deduce their applicability to the review with non-relevant papers being filtered out.

The results of this study highlighted the massive variety in the number of methods used. Most studies focused on either the i7 PCBs or WHO12 PCBs, but many methods included a subset of different PCBs (Figure 1). In terms of instrumentation used, trends show that GC-qMS is the most popular technique among researchers (35% of studies since 2010). GC-ECD use appears to be declining although it is still widely used (21% of studies since 2010) as is GC-HRMS (20% of studies since 2010). Tandem mass spectrometry has seen the greatest increase in use (5% from 2010-14, to 17% from 2014-18) whereas multidimensional techniques are still rarely used (less than 3% of studies since 2010).

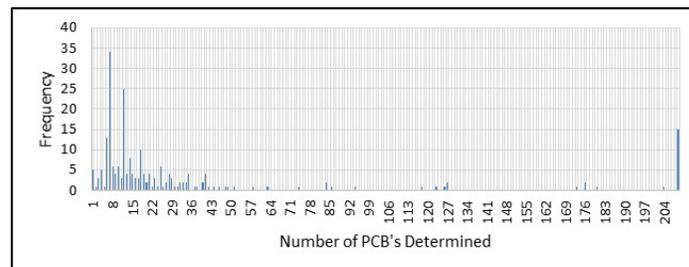


Figure 1: The amounts of PCB's detected/analysed in the literature between 2010 – 2017.

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GeoChem Metrix, Inc. (GCM) is INEF 2018 Chair, Dr. Glenn Johnson's consulting company. Typical GCM projects involve chemical fingerprinting and statistical analysis of environmental data, in support of litigation or cost allocation. GCM also offers training in statistics, chemometrics, environmental forensics and environmental chemistry. Dr. Johnson has authored numerous papers and book chapters on sources, fate and transport of POPs, and numerical methods in environmental forensics. Contact us at 801-571-9372 or info@gcmetrix.com.



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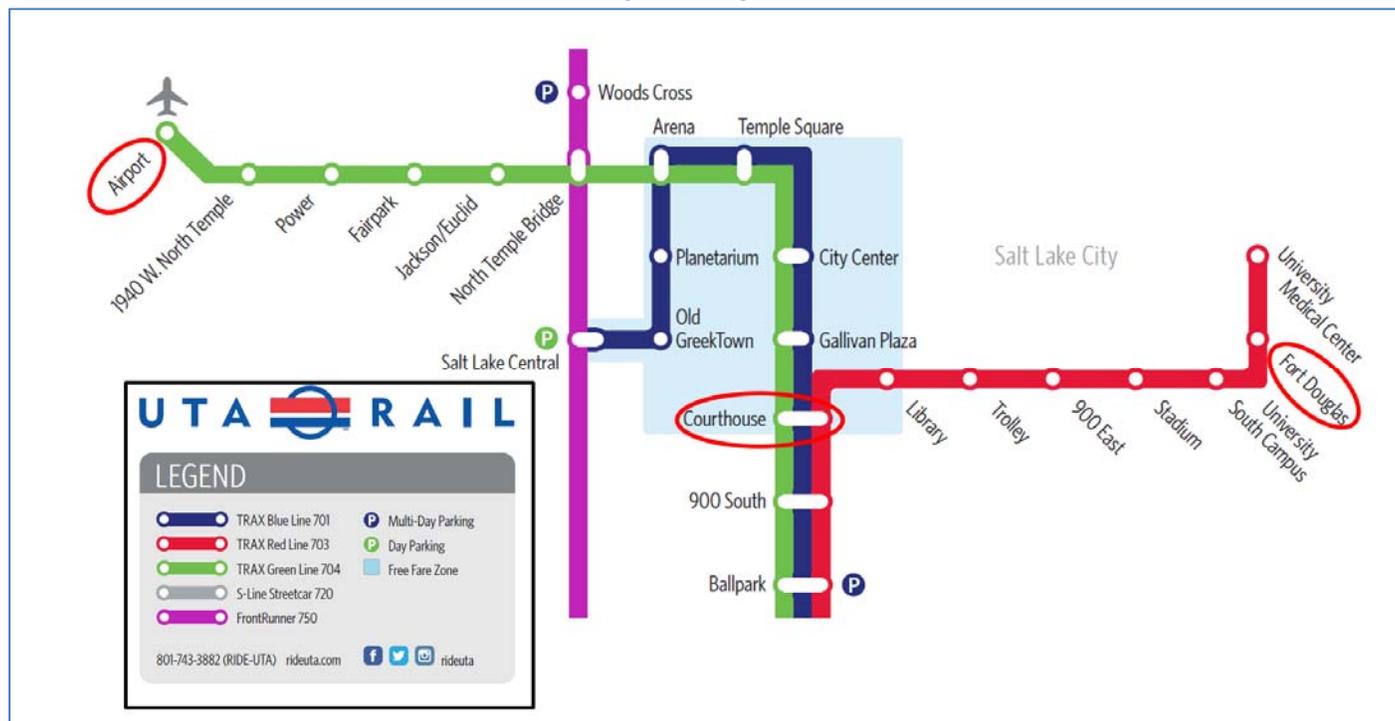


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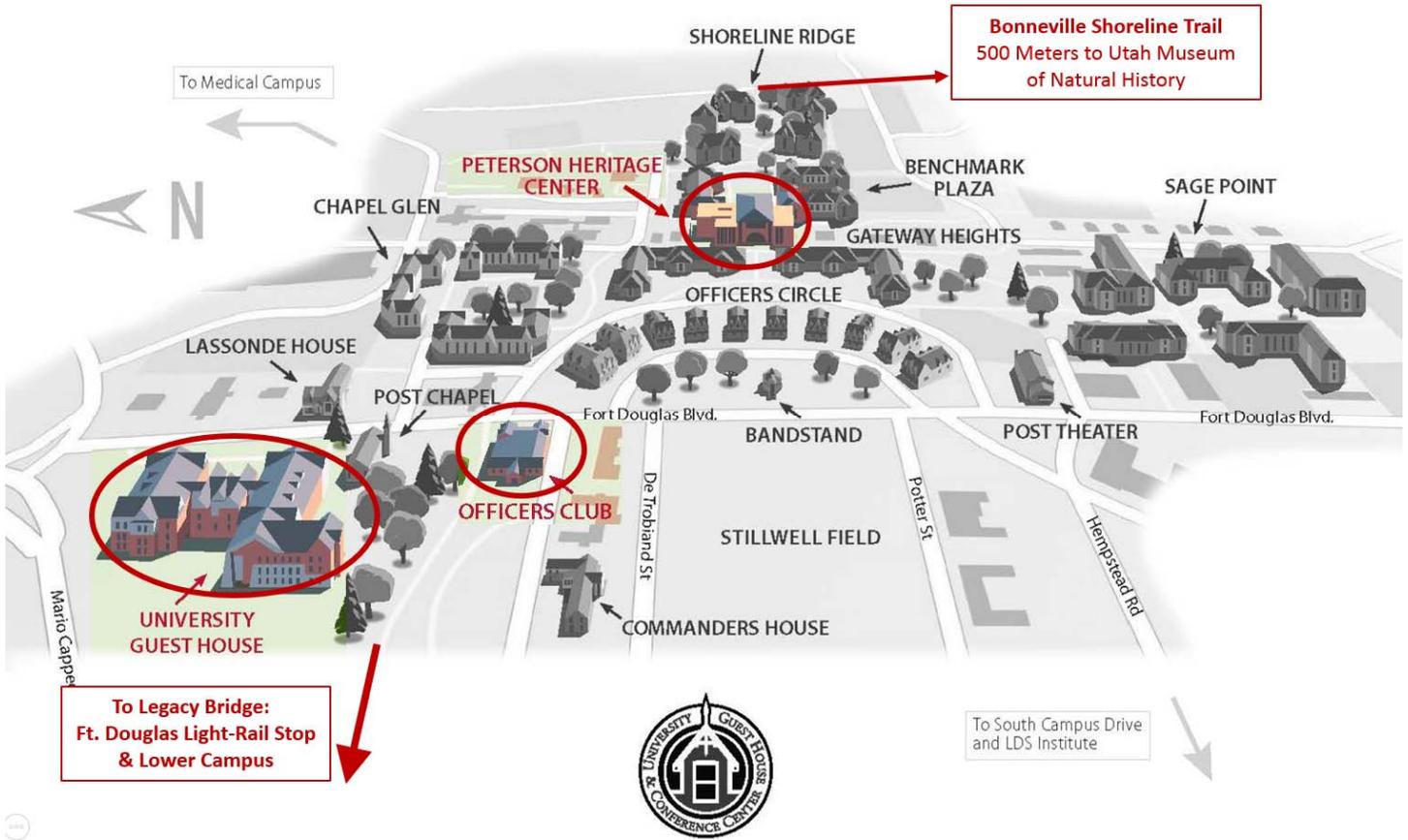
Chemistry Matters Inc. is a boutique environmental consulting firm based in Calgary, Alberta, Canada. Specializing in geoforensics, environmental forensics, biomonitoring and arson investigations, Chemistry Matters provides expert environmental and chemistry consulting services to a variety of clients and industries. With services that are founded on chemistry principles and proper application of scientific methods, Chemistry Matters often provides expert support and expert witness services to projects involving litigious subjects. Learn more about Chemistry Matters at <http://www.chemistry-matters.com>.

LIGHT RAIL (TRAX) SYSTEM MAP



Airport, Fort Douglas (INEF Venue) and Courthouse (Downtown) Stops Highlighted
Full System map at https://www.rideuta.com/~media/RideUTA/Maps/UTA_RAIL_Map.ashx

MAP OF FORT DOUGLAS, UNIVERSITY OF UTAH



MAP OF OFFICERS CLUB LAYOUT FOR INEF 2018

