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MONDAY AFTERNOON

Environmental Science and Technology: A Tribute to William "Bill" Glaze

J. L. Gardea-Torresdey, *Organizer, Presiding*

1:30 —36. Legacy chemicals' legacy. **D. L. Swackhamer**

1:55 —37. Kinetics, mechanisms and stereoselective metabolism of 1,2,4-triazole fungicides in hepatic microsomes and implications for human health and ecological risk assessment. **J. F. Kenneke**, C. S. Mazur, W. M. Henderson, A. W. Garrison, S. E. Ritger, R. D. Miller, T. J. Sack, C. C. Brown, J. K. Avants

2:20 —38. History of the drinking water mutagen MX. **L. Kronberg**, B. Holmbom

2:45 — Intermission.

3:00 —39. Application of an improved pseudo-deterministic receptor model to apportion ambient PM constituents to sources in Tampa, FL. **G. M. Beachley**, J. M. Ondov

3:25 —40. Treatment of truck-wash water using electrocoagulation. **J. A. Gomes**, K. Das, M. S. Rahman, S. Arslan, D. L. Cocke

3:50 —41. Destruction of cyanotoxins by hydroxyl radicals and sulfate radicals: Reaction intermediates and pathways. M. G. Antoniou, J. A. Shoemaker, A. A. de la Cruz, **D. D. Dionysiou**

ABSTRACTS

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Legacy chemicals' legacy

Deborah L. Swackhamer, *dswack@cccs.umn.edu, Environmental Health Sciences, University of Minnesota, Mayo Mail Code 807, 420 Delaware St. SE, Minneapolis, MN 55455, Fax: 612-626-0650*

Our environment was found to be contaminated with PCBs and other persistent, bioaccumulative and toxic chemicals (PBTs) a half-century ago. The Great Lakes was one of the first sites to be studied to understand PBT fate, transport, and effects, and it continues to be a natural laboratory for understanding legacy contaminants as well as chemicals of emerging concern. Our recent work on evaluating the recovery of the Great Lakes from legacy PBTs indicates that the concentrations of banned contaminants have not decreased in sentinel fish species for about 20 years. This is likely due to the continued reservoirs of PBTs in the global atmosphere and in sediments, causing water concentrations (and fish concentrations) to approach steady state. This presents an ecological and human health threat for many decades to come. Given the large numbers of contaminants of emerging concern, a new approach to chemical management is needed.

ENVR 37

Kinetics, mechanisms and stereoselective metabolism of 1,2,4-triazole fungicides in hepatic microsomes and implications for human health and ecological risk assessment

John F. Kenneke¹, *kenneke.john@epa.gov, Christopher S. Mazur*¹, *mazur.chris@epa.gov, W. Matthew Henderson*¹, *henderson.matt@epa.gov, A. Wayne Garrison*¹, *garrison.wayne@epa.gov, Susan E. Ritger*², *ritger.susan@epa.gov, Rebecca D. Miller*³, *miller.rebecca@epa.gov, Thomas J. Sack*⁴, *Cather C. Brown*⁵, and *Jimmy K. Avants*⁴. (1) National Exposure Research Laboratory, U.S. Environmental Protection Agency, 960 College Station Rd, Athens, GA 30605, Fax: 706-355-8202, (2) Student Services Authority, 960 College Station Rd, Athens, GA 30605, (3) Student Services Authority, (4) Senior Service America Incorporated, 960 College Station Rd, Athens, GA 30605, (5) Senior Service America Incorporated

The 1,2,4-triazole fungicides (*i.e.*, conazoles) are potent cytochrome P450 (CYP) modulators and have been used extensively for the control of agricultural and medicinal fungal infections. Recently, emphasis has been placed on the potential adverse effects of these compounds on mammalian steroid biosynthesis and subsequent endocrine system disruption and tumor formation. We have utilized specific enzyme inhibitors,

human CYPs, stable isotopes, stereoselective transformations, molecular docking and in silico modeling to elucidate the mechanisms and kinetics of conazole metabolism in numerous vertebrate and invertebrate species, including humans. The entire paradigm, from delineating the kinetics and mechanisms of xenobiotic transformations to PBPK model development, has been used to improve human health and ecological risk assessment. Results will be presented that illustrate the different approaches and techniques used for studying xenobiotic transformations in biological systems and how experimental results are used to improve risk assessment while reducing the reliance upon *in vivo* animal tests.

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History of the drinking water mutagen MX

Leif Kronberg, *leif.kronberg@abo.fi*, Laboratory of Organic Chemistry, Abo Akademi University, Biskopsgatan 8, FI-20500 Abo/Turku, Finland, Fax: 358-2-2154866, and **Bjarne Holmbom**, *bjarne.holmbom@abo.fi*, Laboratory of Wood and Paper Chemistry, Abo Akademi University, Porthansgatan 3, FI-20500 Abo/Turku, Finland

An historical overview is given of the work on the chlorinated furanone MX, originally called mutagen X. The topics to be presented cover the original work concerning the mutagenicity of chlorine bleached pulp mill effluents and the isolation and identification of the major mutagen (MX), the work on identification of MX in chlorine disinfected drinking water, actions taken by waterworks to minimize the formation of MX and the current state of the work on MX. In the study on mutagenic compounds in pulp mill effluents, MX was isolated in trace amounts and a structure for the compound was suggested. Later, this structure was verified through the synthesis of MX. Subsequently, work on the mutagenicity of chlorine disinfected drinking water was initialized and, through effect-directed analysis, it could be shown that MX was also the major mutagen in drinking water. These findings prompted waterworks to put efforts on finding treatment methods that reduced the content on water dissolved organic material forming MX upon reaction with chlorine or on the use of alternative disinfection methods (e.g., ozonation and chloramine treatment). But still one finds reports on very high concentrations of MX in drinking water.

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Application of an improved pseudo-deterministic receptor model to apportion ambient PM constituents to sources in Tampa, FL

Gregory M. Beachley, *beachlgm@umd.edu* and **John M. Ondov**, Department of Chemistry, University of Maryland, College Park, MD 20742

In 2005, Park *et al.*, developed a new pseudo-deterministic receptor model (PDRM) to apportion SO₂ and ambient particulate matter (PM) constituents to local sources near Tampa Bay. Ambient pollutant measurements were fit to products of emission rates and

dispersion factors constrained with a Gaussian plume model for individual sources. In our study, the original samples were reanalyzed by ICPMS for eight additional elements to improve the resolving power. Chemical mass balance (CMB) terms were added to PDRM to allow fitting of background aerosol sources. More accurate, curvilinear trajectories were computed to predict plume arrival times in both surface and aloft layers. Lastly, predicted emission rates for particle-bound elements were constrained using published source emission profiles. Results show improved fits for 8 of 10 elements and improved emission rates predictions, suggesting that the measurement and PDRM approach represents a viable alternative to expensive stack sampling for developing emission inventories.

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Treatment of truck-wash water using electrocoagulation

Jewel Andrew Gomes¹, *jagomes@my.lamar.edu*, **Kamol Das**², *kamoldas@yahoo.com*, **Md. Sanohar Rahman**², *mailbidut@yahoo.com*, **Sonmez Arslan**¹, *arslanatlar@hotmai.com*, and **David L. Cocke**¹, *dlcocke@my.lamar.edu*. (1) *Department of Chemical Engineering, Lamar University, 4400 MLK Parkway, P.O. Box 10053, Beaumont, TX 77710, Fax: 409-880-8374*, (2) *Department of Civil Engineering, Lamar University, 4400 MLK Parkway, P.O. Box 10053, Beaumont, TX 77710*

With increasing globalization set-up and advances in road transport system, the use and number of heavy duty vehicles, such as trucks, has increased for transportation purposes. Eventually, the wastewater generated due to truck washing has also escalated. This wastewater may impact the environment in various ways. Many particles and chemicals, such as chlorinated solvents, detergents, lubricants, additives, heavy metals, antifreeze, and acid/alkaline wastes have been found in truck-wash waters. The Environmental Protection Agency (EPA) found many washed-off pollutants to be in excess of primary and secondary maximum contaminant levels (MCLs). EPA also raised concern on the issues of TSS, pH, salts, particulate matter, oil, grease, organics, and COD in vehicular wash waters. Another issue is anionic surfactants, such as LAS or linear alkylbenzenesulfonates that are very slow to biodegrade, and have carcinogenic and reproductively toxic by-products. It is necessary to minimize or eliminate potential aesthetic, physical, chemical and biological threats of truck washing waters. At present, several physical and chemical techniques are being used for the treatment of truck-wash water. In this paper, we present our water remediation study on this problem water using electrocoagulation. This accelerated corrosion process includes electrochemistry, surface chemistry, and also physical phenomena. This study shows very efficient removal of metal ions, organics and COD from the truck wash water. The floc that is produced during this treatment has been also characterized using XRD, SEM/EDS, and FT-IR.

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Destruction of cyanotoxins by hydroxyl radicals and sulfate radicals: Reaction intermediates and pathways

Maria G. Antoniou¹, antonim@email.uc.edu, Jody A. Shoemaker², shoemaker.jody@epa.gov, Armah A. de la Cruz², delacruz.armah@epamail.epa.gov, and Dionysios D. Dionysiou¹, dionysios.d.dionysiou@uc.edu. (1) Department of Civil and Environmental Engineering, University of Cincinnati, 765 Baldwin Hall, Cincinnati, OH 45221-0071, Fax: 513-556-2599, (2) Office of Research and Development, U.S. Environmental Protection Agency, 26 W. Martin Luther King Dr, MS 564, Cincinnati, OH 45268

Cyanotoxins, emerging drinking water contaminants, found mainly in surface waters, exhibit acute and chronic lethal toxicity even at significantly low concentrations ($LD_{50} < 100 \mu\text{g}/\text{kg}$ body weight). We are currently evaluating various advanced oxidation technologies (AOTs) for their potential to destroy recalcitrant contaminants such as the cyanotoxins. We have employed oxidants, catalyst and radiation to generate hydroxyl and sulfate radicals to achieve the degradation of the hepatotoxin, microcystin-LR (MC-LR). In this study, we focused on the formation of reaction intermediates with the two types of radicals. It is well known that sulfate radicals have comparable redox potential to hydroxyl radicals but the latter react with organic bonds non-selectively. For these reasons, we identified the chemical structures of the forming reaction intermediates for each type of radical and compared the degradation routes and preferential sites of attack. For the structural elucidation of the intermediates, tandem mass spectrometry (MS/MS) was utilized.