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# Using a Statistical Technique To Test PATHOGENS in WATER

Coupling Engineering and Science
To Prevent Bioaerosol-Related Disease

Examining the Effects of Low-Level
Pesticide Mixtures on Wild Salmon

PUBLISHED BY THE AMERICAN CHEMICAL SOCIETY

#### Research

#### **CRITICAL REVIEW**

#### 4639

Critical Review: Life-Cycle Inventory Procedures for Long-Term Release of Metals

Johan Pettersen\* and Edgar G. Hertwich

Issues concerning applicability and possible risk perspectives in life-cycle assessment for current and alternative approaches for inorganic leaching potential are discussed.

#### **POLICY ANALYSIS**

#### 4648

Policies for Chemical Hazard and Risk Priority Setting: Can Persistence, Bioaccumulation, Toxicity, and Quantity Information Be Combined?

Jon A. Arnot\* and Don Mackay

The advantages of combining persistence, bioaccumulation, toxicity and quantity information for chemical assessments are explored.

#### 4655

Brown Superfund Basic Research Program: A
Multistakeholder Partnership Addresses Real-World Problems
in Contaminated Communities

Laura Senier,\* Benjamin Hudson, Sarah Fort, Elizabeth Hoover, Rebecca Tillson, and Phil Brown

This case study demonstrates how research translation and outreach activities that are clearly differentiated and well-integrated can improve a basic and applied research program.

#### 4663

#### ► Assessing the End-of-Life Impacts of Buildings

Pedro Santos Vieira and Arpad Horvath\*

Theories on end of life of products are synthesized, and a method for environmental decision-making related to buildings is presented.

#### 4670

## Current and Future Linked Responses of Ozone and $PM_{2.5}$ to Emission Controls

Kuo-Jen Liao, Efthimios Tagaris, Sergey L. Napelenok, Kasemsan Manomaiphiboon, Jung-Hun Woo, Praveen Amar, Shan He, and Armistead G. Russell\*

Daily pollutant responses to emission changes suggest that strategies developed to meet standards should consider other air quality impacts.

#### 4676

#### An Assessment of Fecal Indicator Bacteria-Based Water Quality Standards

Andrew D. Gronewold,\* Mark E. Borsuk, Robert L. Wolpert, and Kenneth H. Reckhow

A novel approach to developing and assessing fecal indicator bacteria-based water quality standards for pathogenically impaired resource waters is presented.

#### 2C ■ ENVIRONMENTAL SCIENCE & TECHNOLOGY / JULY 1, 2008

# CHARACTERIZATION OF NATURAL AND AFFECTED ENVIRONMENTS

#### 4683

## Nitrate Contamination in Groundwater on an Urbanized Dairy Farm

William J. Showers,\* Bernard Genna, Timothy McDade, Rick Bolich, and John C. Fountain

Multiple stable isotopes and chloride/bromide ratios indicate groundwater nitrate contamination on an urbanized dairy farm is from pasture wastes and not septic failures.

#### 4689

#### Trimethylamine as Precursor to Secondary Organic Aerosol Formation via Nitrate Radical Reaction in the Atmosphere

Philip J. Silva,\* Mark E. Erupe, Derek Price, John Elias, Quentin G. J. Malloy, Qi Li, Bethany Warren, and David R. Cocker III

Ambient and smog chamber experiments showing the potential of trimethylamine as a precursor to secondary organic aerosol are described.

#### 4697

#### Carbonyl Emissions from Gasoline and Diesel Motor Vehicles

Chris A. Jakober, Michael A. Robert, Sarah G. Riddle, Hugo Destaillats, M. Judith Charles, Peter G. Green, and Michael J. Kleeman\*

Carbonyl compounds present in motor vehicle exhaust, ranging from  $C_2$  to  $C_{13}$ , comprise a substantial fraction of light-duty gasoline vehicle particulate matter emissions.

#### **4704**

# Brominated Flame Retardants, Polychlorinated Biphenyls, and Organochlorine Pesticides in Captive Giant Panda (*Ailuropoda melanoleuca*) and Red Panda (*Ailurus fulgens*) from China

Guo-Cheng Hu, Xiao-Jun Luo, Jia-Yin Dai,\* Xiu-Lan Zhang, Hua Wu, Cheng-Lin Zhang, Wei Guo, Mu-Qi Xu, Bi-Xian Mai,\* and Fu-Wen Wei

The concentrations of chlorinated and brominated contaminants are measured in tissue samples from captive giant pandas and red pandas in China.

#### 4710

#### Mercury Deposition in a Polar Desert Ecosystem

Rebecca A. Witherow\* and W. Berry Lyons

Sources of mercury to snow in Victoria Land, Antarctica and the transport of mercury to glacial meltwater streams are discussed.

#### 4717

#### U, Pu, and Am Nuclear Signatures of the Thule Hydrogen Bomb Debris

Mats Eriksson,\* Patric Lindahl, Per Roos, Henning Dahlgaard, and Elis Holm This article describes the nuclear signature of environmentally

This article describes the nuclear signature of environmental released hot particles and discussion on the preferential leaching of uranium relative to plutonium in this environment.

#### **4723**

#### Isotope and Ion Selectivity in Reverse Osmosis Desalination: Geochemical Tracers for Man-made Freshwater

Wolfram Kloppmann,\* Avner Vengosh, Catherine Guerrot, Romain Millot, and Irena Pankratov

The isotope fingerprints (B, Li, Sr, O, H) and ion selectivity of reverse osmosis desalination are investigated in commercial desalination plants.

#### **4732**

#### Seven Thousand Years of Records on the Mining and Utilization of Metals from Lake Sediments in Central China

Celine S. L. Lee, Shi-hua Qi, Gan Zhang, Chun-ling Luo, Lu Y. L. Zhao, and Xiang-dong Li\*

Direct evidence of environmental influences of mining and utilization of metals in the last 7,000 years in China is provided.

#### **4739**

#### Temporal Trends of Perfluoroalkyl Compounds with Isomer Analysis in Lake Trout from Lake Ontario (1979–2004)

Vasile I Furdui,\* Paul A. Helm, Patrick W. Crozier, Corina Lucaciu, Eric J. Reiner, Chris H. Marvin, D. Michael Whittle, Scott A. Mabury, and Gregg T. Tomy

Isomer-specific analysis revealed the presence of branched perfluorocarboxylates with a shifting trend toward the exclusive occurrence of linear isomers in recent samples.

#### 4745

#### Flame Retardants in the Atmosphere near the Great Lakes

Marta Venier and Ronald A. Hites\*

Concentrations of BDE-47 and BDE-99, which are representative of the banned penta-mixture, are decreasing over time, whereas BDE-209, the main constituent of the unregulated deca-mixture, is not.

#### **ENVIRONMENTAL PROCESSES**

#### **4752**

#### Dechlorination of Tetrachloroethylene in Aqueous Solutions Using Metal-Modified Zerovalent Silicon

Chun-chi Lee and Ruey-an Doong\*

The combination of Ni(II) with Si(0) is an environmentally friendly reductant to enhance the hydrodechlorination efficiency and rate of tetrachloroethylene.

#### 4758

## Octachlorodibenzodioxin Formation on Fe(III)-Montmorillonite Clay

Cheng Gu, Hui Li, Brian J. Teppen, and Stephen A. Boyd\*

Direct evidence is provided for clay-catalyzed formation of octachlorodibenzodioxin supporting the plausibility of its in situ formation in soils, subsoils, and clay deposits.

#### 4764

#### Identifying Competing Aerobic Nitrobenzene Biodegradation Pathways by Compound-Specific Isotope Analysis

Thomas B. Hofstetter,\* Jim C. Spain,\* Shirley F. Nishino, Jakov Bolotin, and René P. Schwarzenbach

<sup>13</sup>C and <sup>15</sup>N enrichment of nitrobenzene during dihydroxylation by *Comamonas* sp. strain JS765 and partial reduction by *Pseudomonas pseudoalcaligenes* strain JS45 are distinctly different.

#### 4771

### Effect of Volatile—Char Interaction on the NO Emission from Coal Combustion

Mingyu Yao, Defu Che,\* Yanhua Liu, and Yinhe Liu

The effect of volatile—char interaction on fuel-N conversion to NO is investigated by separate combustion of volatile and char and by entrained pulverized coal combustion.

#### **4777**

#### Confounding Impacts of Iron Reduction on Arsenic Retention

Katharine J. Tufano and Scott Fendorf\*

Iron (hydr)oxide reduction has confounding impacts on arsenic retention, increasing arsenic retention during active transformation (dissolution—reprecipitation) but decreasing retention during dissolution.

#### **4784**

## Adaptation of Aerobic, Ethene-Assimilating *Mycobacterium* Strains to Vinyl Chloride as a Growth Substrate

Yang Oh Jin and Timothy E. Mattes\*

Four ethene-degrading *Mycobacterium* strains began utilizing vinyl chloride, a common groundwater pollutant, as a growth substrate after extended incubation periods.

#### 4790

## Isomer-Specific Biodegradation of Methylphenanthrenes by Soil Bacteria

Rasmus F. Lamberts, Jan H. Christensen, Philipp Mayer, Ole Andersen, and Anders R. Johnsen\*

Soil bacteria show no general preference for 2-methylphenanthrene compared to 1-methylphenanthrene; however, individual isolates may be isomer specific.

#### 4797

## Interactions of Hydrophobic Fractions of Dissolved Organic Matter with $Fe^{3+}$ - and $Cu^{2+}$ -Montmorillonite

Tamara Polubesova, Yona Chen, Rotem Navon, and Benny Chefetz\*

Montmorillonite enriched with  $Fe^{3+}$  enhanced adsorption and fractionation of hydrophobic fractions of dissolved organic matter.

#### **ENVIRONMENTAL MODELING**

#### 4804

#### Modeling Arsenic in the Patuxent Estuary

Alex J. Nice, Wu-Seng Lung,\* and Gerhardt F. Riedel

A water quality model is developed to track the fate and transport of for arsenic species in the Patuxent Estuary.

#### 4811

#### Degradation of Tertiary Alkylamines during Chlorination/ Chloramination: Implications for Formation of Aldehydes, Nitriles, Halonitroalkanes, and Nitrosamines

William A. Mitch\* and I. Marie Schreiber

Chlorination and chloramination of tertiary alkylamines rapidly forms significant concentrations of secondary amines and aldehydes, with very low yields of nitrogenous byproducts.

#### 4818

#### Nowcasting and Forecasting Concentrations of Biological Contaminants at Beaches: A Feasibility and Case Study

Walter E. Frick,\* Zhongfu Ge, and Richard G. Zepp

The Virtual Beach tool is used to develop statistical models for dynamic nowcasting and forecasting of *Escherichia coli* levels at a Great Lakes beach.

#### 4825

#### Effect of Pore-Blocking Background Compounds on the Kinetics of Trace Organic Contaminant Desorption from Activated Carbon

Priscilla C. To, Benito J. Mariñas,\* Vernon L. Snoeyink, and Wun Jern Ng

The effect of competition by pore blocking background organic matter on decreasing the desorption kinetics of a trace contaminant is explored.

#### **4831**

Modeling the Importance of Biota and Black Carbon As Vectors of Polybrominated Diphenyl Ethers (PBDEs) in the Baltic Sea Ecosystem

Tuomas J. Mattila\* and Matti Verta

Influence of aquatic biota and black carbon to PBDE transport is studied with a multimedia mass balance model of the Baltic Sea.

#### **ENVIRONMENTAL MEASUREMENTS METHODS**

#### 4837

The Effects of Dual-Domain Mass Transfer on the Tritium—Helium-3 Dating Method

Rebecca B. Neumann, Eric M. LaBolle, and Charles F. Harvey\*

Diffusion of tritiated water and helium-3 between mobile and immobile regions in aquifers can dramatically affect tritium—helium-3 ages, producing anomalous behaviors that are consistent with a variety of data sets.

#### **4844**

NMR Determination of Total Carbonyls and Carboxyls: A Tool for Tracing the Evolution of Atmospheric Oxidized Organic Aerosols

F. Moretti,\* E. Tagliavini, S. Decesari, M. C. Facchini, M. Rinaldi, and S. Fuzzi

Chemical derivatization coupled with <sup>1</sup>H NMR spectroscopy provides quantitative analysis of functional groups including carbonyls and carboxylic acid in atmospheric organic aerosol samples.

#### **4850**

A Plume Capture Technique for the Remote Characterization of Aircraft Engine Emissions

G. R. Johnson, M. Mazaheri, Z. D. Ristovski, and L. Morawska\*

An approach is described for measuring particle size distributions and emission factors using transient plumes such as the exhaust of a jet aircraft.

#### 4857

#### Formation of *N*-Nitrosamines from Eleven Disinfection Treatments of Seven Different Surface Waters

Yuan-Yuan Zhao, Jessica M. Boyd, Matthew Woodbeck, Robert C. Andrews, Feng  $\Omega$ in, Steve E. Hrudey, and Xing-Fang Li\*

Formation of nine *N*-nitrosamines from eleven treatments of seven different source waters without addition of any precursors is investigated.

#### 4863

#### Comparison of Selection Methods To Deduce Natural Background Levels for Groundwater Units

Jasper Griffioen,\* Hilde F. Passier, and Janneke Klein

Selection of groundwater samples is an essential step in deducing natural background levels for groundwater units, and a combination of methods provides internal control.

#### **4870**

Novel Chamber to Measure Equilibrium Soil—Air Partitioning Coefficients of Low-Volatility Organic Chemicals under Conditions of Varying Temperature and Soil Moisture

André Wolters,\* Volker Linnemann, Kilian E. C. Smith, Eva Klingelmann, Byung-Jun Park, and Harry Vereecken

Soil–air partitioning of very low-volatility compounds is measured by a highly precise method that even allows quantitation of temperature and soil moisture effects.

#### 4877

Underpotential Deposition—Anodic Stripping Voltammetric Detection of Copper at Gold Nanoparticle-Modified Ultramicroelectrode Arrays

Jahir Orozco,\* César Fernández-Sánchez, and Cecilia Jiménez-Jorquera

The sensitive UPD-ASV detection of copper (II) in soil samples using gold nanoparticle-modified UMEAs is described.

#### REMEDIATION AND CONTROL TECHNOLOGIES

#### 4883

Surfactants as Bubble Surface Modifiers in the Flotation of Algae: Dissolved Air Flotation That Utilizes a Chemically Modified Bubble Surface

Rita K. Henderson, Simon A. Parsons, and Bruce Jefferson\*

Dosing surfactants into the saturator system of a dissolved air flotation process provides a means of enhancing algae removal without the need for coagulation.

#### 4889

## Ozonation of Ciprofloxacin in Water: HRMS Identification of Reaction Products and Pathways

Bavo DeWitte, Jo Dewulf,\* Kristof Demeestere, Vincent Van De Vyvere, Patrick De Wispelaere, and Herman Van Langenhove

Ozonation of ciprofloxacin at different pH and  $\rm H_2O_2$  conditions is studied, and degradation intermediates and pathways are proposed based on HRMS identification.

#### **4896**

## Reduced Toxicity of Olive Mill Waste Waters by Oxidative Coupling with Biomimetic Catalysis

Giuseppe Celano, Daniela Šmejkalová, Riccardo Spaccini, and Alessandro Piccolo\*

Reduced toxicity of waste waters by biomimetic catalysis.

#### 4902

## Hydrothermal Synthesis and Photocatalytic Activity of Zinc Oxide Hollow Spheres

Jiaguo Yu\* and Xiaoxiao Yu

ZnO hollow spheres are fabricated by a hydrothermal and calcination method and their textures and photoactivity can be tuned by varying composition of reactant.

#### 4908

#### Sensitizers on Inorganic Carriers for Decomposition of the Chemical Warfare Agent Yperite

Bogdan Cojocaru, Vasile I. Parvulescu,\* Elena Preda, Gabriel Iepure, Vasile Somoghi, Esther Carbonell, Mercedes Alvaro, and Hermenegildo García

Efficient photocatalytic decomposition of yperite was achieved using heterogeneous photocatalysts consisting of a metal phthalocyanine or 2,4,6-triphenylpyrylium encapsulated inside the cavities of microporous or mesoporous channels.

#### **4914**

#### Essential Explanation of the Strong Mineralization Performance of Boron-Doped Diamond Electrodes

Xiuping Zhu, Meiping Tong, Shaoyuan Shi, Huazhang Zhao, and Jinren Ni\*

The essential mechanism resulting in a high mineralization performance of BDD anodes is that hydroxyl radicals mainly exist as free hydroxyl radicals at BDD anodes.

#### ■ 4921

#### Polyoxometalate-Enhanced Oxidation of Organic Compounds by Nanoparticulate Zero-Valent Iron and Ferrous Ion in the Presence of Oxygen

Changha Lee, Christina R. Keenan, and David L. Sedlak\*

Polyoxometalate greatly increases the yield of oxidants from nanoparticulate zero-valent iron and ferrous ion by serving as an electron shuttle and an iron-chelating agent.

#### ■ 4927

#### Bactericidal Effect of Zero-Valent Iron Nanoparticles on Escherichia coli

Changha Lee, Jee Yeon Kim, Won II Lee, Kara L. Nelson, Jeyong Yoon,\* and David L. Sedlak\*

In the absence of oxygen, the cell membranes of *E. coli* undergo physical disruption, leading to inactivation upon exposure to low concentrations of iron nanoparticles.

#### 4934

## Design of BDD-TiO<sub>2</sub> Hybrid Electrode with P—N Function for Photoelectrocatalytic Degradation of Organic Contaminants

Jiuhui Qu\* and Xu Zhao

P-N hybrid electrode of boron-doped diamond and  $TiO_2$  is designed and fabricated, which exhibits high photoelectrocatalytic activities toward degradation of acid orange II and 2,4-dichlorophenol.

#### 4940

## Pretreatment of Hanford Medium-Curie Wastes by Fractional Crystallization

Laurent Nassif, George Dumont, Hatem Alysouri, Ronald W. Rousseau,\* and Don Geneisse

Research involving simulated wastes has shown that fractional crystallization is a potentially viable method for accelerating treatment of Hanford wastes.

#### ■ 4946

#### Degradation of Lead-Contaminated Lignocellulosic Waste by Phanerochaete chrysosporium and the Reduction of Lead Toxicity

Dan-Lian Huang, Guang-Ming Zeng,\* Chong-Ling Feng, Shuang Hu, Xiao-Yun Jiang, Lin Tang, Feng-Feng Su, Yu Zhang, Wei Zeng, and Hong-Liang Liu

The degradation of Pb-polluted lignocellulosic waste and the alleviation of Pb hazards by fungus *Phanerochaete chrysosporium* were demonstrated.

# SUSTAINABILITY ENGINEERING AND GREEN CHEMISTRY

#### **4952**

## Photoreactive TiO<sub>2</sub>/Carbon Nanotube Composites: Synthesis and Reactivity

Yuan Yao, Gonghu Li, Shannon Ciston, Richard M. Lueptow, and Kimberly A. Gray\*

A composite material of 100 nm anatase phase  ${\rm TiO_2}$  and single-walled carbon nanotubes exhibits reduced charge recombination and enhanced photoreactivity.

#### 4958

#### Model-Centered Approach to Early Planning and Design of an Eco-Industrial Park around an Oil Refinery

Xiangping Zhang, Anders H. Strømman, Christian Solli, and Edgar G. Hertwich\*

The integration of a combined heat and power plant, a synfuel plant, aquaculture, and CO<sub>2</sub> capture and storage are proposed for a refinery in Mongstad, Norway.

#### **4964**

## Efficiency Dilution: Long-Term Exergy Conversion Trends in Japan

Eric Williams,\* Benjamin Warr, and Robert U. Ayres

Long-term exergy efficiency trends in Japan are assessed, showing that while individual technologies tend to improve, aggregate efficiency can even decline as less exergy-efficient technologies are added to the mix.

#### 4971

#### Activated Carbon Cloth as Anode for Sulfate Removal in a Microbial Fuel Cell

Feng Zhao, Nelli Rahunen, John R. Varcoe, Amreesh Chandra, Claudio Avignone-Rossa, Alfred E. Thumser, and Robert C. T. Slade\*

Employing activated carbon cloth as anode, a microbial fuel cell demonstrated high-efficiency sulfate removal and simultaneously high power output.

#### 4977

#### Exergy Analysis of Integrated Waste Management in the Recovery and Recycling of Used Cooking Oils

Laura Talens Peiró, Gara Villalba Méndez,\* and Xavier Gabarrell i Durany

This paper accounts for the potential reduction of exergy loss and also shows how increasing the collection of oils provides a sustainable process for biodiesel production.

# ECOTOXICOLOGY AND HUMAN ENVIRONMENTAL HEALTH

#### ■ 4982

## Copper Oxide-Based Model of Persistent Free Radical Formation on Combustion-Derived Particulate Matter

Slawo Lomnicki, Hieu Truong, Eric Vejerano, and Barry Dellinger\*

Environmentally persistent free radicals are formed by chemisorption of substituted phenols and chlorobenzenes to copper(II) oxide-containing particles followed by electron transfer and reduction to Cu(I).

#### **4989**

#### ► Decline in Perfluorooctanesulfonate and Other Polyfluoroalkyl Chemicals in American Red Cross Adult Blood Donors, 2000—2006

Geary W. Olsen,\* David C. Mair, Timothy R. Church, Mark E. Ellefson, William K. Reagen, Theresa M. Boyd, Ross M. Herron, Zahra Medhdizadehkashi, John B. Nobiletti, Jorge A. Rios, John L. Butenhoff, and Larry R. Zobel

Several years after a primary manufacturer's phase-out of POSF-based materials, concentrations of PFOS and other polyfluoroalkyl chemicals are declining in adult blood donors.

#### 4996

## Salmon Olfaction is Impaired by an Environmentally Realistic Pesticide Mixture

Keith B. Tierney, Jessica L Sampson, Peter S. Ross, Mark A. Sekela, and Christopher J. Kennedy\*

An environmentally realistic concentration of a pesticide mixture alters the ability of the common salmonid rainbow trout to detect a behaviorally important odorant.

#### 5002

## Alveolar Air and Urine Analyses As Biomarkers of Exposure to Trihalomethanes in an Indoor Swimming Pool

J. Caro and M. Gallego\*

A systematic and concurrent study is carried out to assess the trihalomethane uptake of workers and swimmers in an enclosed swimming facility.

#### **5008**

## High Percentage Inorganic Arsenic Content of Mining Impacted and Nonimpacted Chinese Rice

Y.-G. Zhu,\* G.-X. Sun, M. Lei, M. Teng, Y.-X. Liu, N.-C. Chen, L.-H. Wang, A. M. Carey, C. Deacon, A. Raab, A. A. Meharg, and P. N. Williams\*

A new rapid speciation extraction for As reveals rice from mine-impacted regions in central and southern China to be elevated in inorganic As.

#### 5014

#### Fenton-Like Reaction Catalyzed by the Rare Earth Inner Transition Metal Cerium

Eric G. Heckert, Sudipta Seal, and William T. Self\*

The rare earth metal cerium is found to produce hydroxyl and superoxide radicals in the presence of hydrogen peroxide in a Fenton-like reaction.

#### **5020**

#### An Environmental Estrogen Alters Reproductive Hierarchies, Disrupting Sexual Selection in Group-Spawning Fish

Tobias S. Coe,\* Patrick B. Hamilton, David Hodgson, Gregory C. Paull, Jamie R. Stevens, Katie Sumner, and Charles R. Tyler

Exposure to ethinylestradiol disrupts natural patterns of parentage and reproductive success in the group-spawning zebrafish *Danio rerio*.

#### **5026**

Ingested Microscopic Plastic Translocates to the Circulatory System of the Mussel, *Mytilus edulis* (L.)

Mark A. Browne,\* Awantha Dissanayake, Tamara S. Galloway, David M. Lowe, and Richard C. Thompson

Ingested particles of microplastic translocate from the gut cavity to the hemolymph and hemocytes of the marine mussel, *Mytilus edulis* (L.).

#### **ADDITIONS AND CORRECTIONS**

#### 5032

The  $pK_a$  Values of PFOA and Other Highly Fluorinated Carboxylic Acids

Kai-Uwe Goss

Supporting information is available free at http://pubs.acs.org/est.
 This research is highlighted in the News and Features section.