POCTOBER 1, 2004

NOTE OF THE POST OF THE

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When SYNTHETIC
 Chemicals Degrade
 in the Environment

Global Assessment of PBDEs in Farmed and Wild Salmon

Azo Dye Method for Mapping Relative Sediment Enzyme Activity

> PUBLISHED BY THE AMERICAN CHEMICAL SOCIETY

### Research

### Characterization of Natural and Affected Environments

#### **4913**

Polychlorinated Naphthalenes in Swedish Background Air

Anna-Lena Egebäck, Ulla Wideqvist, Ulf Järnberg, and Lillemor Asplund

This study examines differences in concentration, congener composition, and gas/particle distribution between southern and northern locations under various weather conditions.

#### 4921

Redox Chemistry in Minnesota Streams during Episodes of Increased Methylmercury Discharge

Steven J. Balogh, Yabing H. Nollet, and Edward B. Swain

Water chemistry data suggest that wetlands were the source of high methylmercury concentrations in two Minnesota streams during a runoff event in July 2003.

#### 4928

Polycyclic Aromatic Hydrocarbon Sources Related to Biomarker Levels in Fish from Prince William Sound and the Gulf of Alaska

David S. Page, Robert J. Huggett, John J. Stegeman, Keith R. Parker, Bruce Woodin, John S. Brown, and A. Edward Bence

Biomarker induction observed in fish from Prince William Sound and the Gulf of Alaska is related to numerous natural and anthropogenic PAH sources.

#### 4937

Source Identification of PCDD/Fs for Various Atmospheric Environments in a Highly Industrialized City

Wei-Shan Lee, Guo-Ping Chang-Chien, Lin-Chi Wang, Wen-Jhy Lee, Perng-Jy Tsai, Kuen-Yuh Wu, and Chieh Lin

In traffic areas, PCDD/F emissions are primarily from vehicles; in industrial areas, emissions are primarily from metallurgical facilities rather than from medical waste incinerators.

#### 4945

#### ► Global Assessment of Polybrominated Diphenyl Ethers in Farmed and Wild Salmon

Ronald A. Hites, Jeffery A. Foran, Steven J. Schwager, Barbara A. Knuth, M. Coreen Hamilton, and David O. Carpenter

PBDEs are more concentrated in farm-raised salmon than in most wild salmon and more concentrated in salmon from farms in Europe than in those from farms in Chile.

#### 4950

Enantiomeric Specificity of Methylsulfonyl-PCBs and Distribution of Bis(4-chlorophenyl) Sulfone, PCB, and DDE Methyl Sulfones in Grey Seal Tissues

Christina Larsson, Karin Norström, Ioannis Athanansiadis, Anders Bignert, Wilfried A. König, and Åke Bergman

Grey seal liver is a significant target tissue, and blubber tissue level cannot be relied upon as the primary indicator of PCB methyl sulfone toxicity.

#### 4956

Investigations into the Vertical Distribution of PCDDs and Mineralogy in Three Ball Clay Cores from the United States Exhibiting the Natural Formation Pattern

Damien Gadomski, Mats Tysklind, Robert L. Irvine, Peter C. Burns, and Rolf Andersson

The vertical distribution and profiles of polychlorinated dioxins and mineralogy in ball clay samples in the United States indicate a possible naturally occurring dechlorination process.

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- Effective January 1, 2005, all ES&T research papers must be submitted via the Web (https://paragon.acs.org/ paragon/index.jsp). Email submissions or paper copies will not be accepted.

#### 4964

Atmospheric Mercury Accumulation Rates Between 5900 and 800 Calibrated Years BP in the High Arctic of Canada Recorded by Peat Hummocks

Nicolas Givelet, Fiona Roos-Barraclough, Michael E. Goodsite, Andriy K. Cheburkin, and William Shotyk

This study presents the first comprehensive long-term record of pre-anthropogenic rates of atmospheric mercury accumulation in dated peat deposits in the High Arctic of Canada.

#### 4973

Gas-Particle Partitioning of Polycyclic Aromatic Hydrocarbons in Urban, Adjacent Coastal, and Continental Background Sites of Western Greece

Eleni Terzi and Constantini Samara

The gas-particle partitioning of atmospheric PAHs at three sites in western Greece indicates deviations from predicted aerosol behavior due to disequilibrium and different particle characteristics.

#### **Environmental Processes**

#### 4979

Kinetics of Trace Metal Competition in the Freshwater Environment: Some Fundamental Characteristics

Ismail I. Fasfous, Tahir Yapici, John Murimboh, Nouri M. Hassan, Chuni L. Chakrabarti, Margaret H. Back, David R. S. Lean, and D. Conrad Grégoire

A study of kinetics of trace metal competition in freshwater has revealed the importance of metal-to-ligand ratio, ionic potential, and ligand field stabilization energy.

#### 4987

Investigation of Sorption Behavior between Pyrene and Colloidal Organic Carbon from Activated Sludge Processes

R. David Holbrook, Nancy G. Love, and John T. Novak

Fluorescence quenching is used to investigate sorption of pyrene by different-sized fractions of colloidal organic carbon originating from two biological wastewater treatment reactors.

#### 4995

Chlorination Byproduct Formation in the Presence of Humic Acid, Model Nitrogenous Organic Compounds, Ammonia, and Bromide

Xin Yang and Chii Shang

Effects are evaluated of the presence of organic nitrogen compounds, ammonia, and bromide on the formation of trihalomethanes, haloacetic acids, and cyanogens halides in chlorinating humic acid solutions.

- Supporting Information is available free of charge via the Internet at http://pubs.acs.org.
- This issue contains a news story about this research.

#### 5002

## Stable Metal Isotopes Reveal Copper Accumulation and Loss Dynamics in the Freshwater Bivalve Corbicula

Marie-Noële Croteau, Samuel N. Luoma, Brent R. Topping, and Cary B. Lopez

Manipulation of copper stable isotopic ratios allows characterization of copper bioaccumulation dynamics (uptake and loss) in a freshwater invertebrate, the bivalve *Corbicula fluminea*.

#### 5010

#### Methylmercury and Total Mercury in Plant Litter Decomposing in Upland Forests and Flooded Landscapes

Britt D. Hall and Vincent L. St. Louis

A litterbag approach is used to examine changes in methylmercury, total mercury, carbon, and nitrogen in 12 plant tissues decomposing in flooded and unflooded forests.

#### 5022

#### Investigations of the Reactions of Monochloramine and Dichloramine with Selected Phenols: Examination of Humic Acid Models and Water Contaminants

Victor L. Heasley, Audra M. Fisher, Erica E. Herman, Faith E. Jacobsen, Evan W. Miller, Ashley M. Ramirez, Nicole R. Royer, Josh M. Whisenand, David L. Zoetewey, and Dale F. Shellhamer

The reactions of several phenols with monochloramine and dichloramine are described, including the displacement of the para-chlorine from trichlorophenols.

#### 5030

#### Using the Biotic Ligand Model for Predicting the Acute Sensitivity of Cladoceran-Dominated Communities to Copper in Natural Surface Waters

Bart T. A. Bossuyt, Karel A. C. De Schamphelaere, and Colin R. Janssen Using both laboratory isolates and field-collected species,

Using both laboratory isolates and field-collected species, researchers applied the biotic ligand model to predict copper toxicity to cladocerans.

#### 5038

# Products and Mechanism of the Reaction of OH Radicals with 2,3,4-Trimethylpentane in the Presence of NO

Sara M. Aschmann, Janet Arey, and Roger Atkinson

A relative rate method is used to determine a rate constant for the gas-phase reaction of OH radicals with 2,3,4-trimethylpentane and to quantify products.

#### 50/6

# Reductive Dechlorination of $\alpha$ -, $\beta$ -, $\delta$ -, and $\gamma$ -Hexachlorocyclohexane Isomers by Hydroxocobalamin in the Presence of Either Dithiothreitol or Titanium(III) Citrate as Reducing Agents

B. Rodríguez-Garrido, M. Camps Arbestain, M. C. Monterroso, and F. Macías

The potential for dehalogenation of hexachlorocyclohexane isomers by hydroxocobalamin in the presence of either dithiothreitol or titanium(III) citrate as reducing agents is investigated.

#### 5053

# Influence of Oxidation States on Plutonium Mobility during Long-Term Transport through an Unsaturated Subsurface Environment

Daniel I. Kaplan, Brian A. Powell, Deniz I. Demirkanli, Robert A. Fjeld, Fred J. Molz, Steven M. Serkiz, and John T. Coates

A lysimeter containing sediment and solid  $Pu^{IV}(NO_3)_4$  left exposed for 11 years reveals that both reduction and oxidation processes play an important role in plutonium transport.

#### Supporting Information is available free of charge via the Internet at http://pubs.acs.org.

#### 5059

#### Identification of Copper Binding Sites in Soil Organic Matter through Chemical Modifications and <sup>13</sup>C CP-MAS NMR Spectroscopy

M. Schilling and W. T. Cooper

<sup>13</sup>C CP-MAS NMR spin-lattice relaxation rates of chemically modified soils doped with paramagnetic Cu<sup>2+</sup> are used to identify copper binding sites in soil organic matter.

#### 5064

#### Formation of Secondary Organic Aerosol by Reactive Condensation of Furandiones, Aldehydes, and Water Vapor onto Inorganic Aerosol Seed Particles

Charles A. Koehler, Jeremiah D. Fillo, Kyle A. Ries, José T. Sanchez, and David O. De Haan

Volatile furandiones and aldehydes form organic aerosol in humid conditions through mechanisms that are dependent on condensed-phase chemical reactions rather than simple partitioning.

#### 5073

#### Natural Perchlorate Has a Unique Oxygen Isotope Signature

Huiming Bao and Baohua Gu

Triple oxygen isotope ratios (<sup>16</sup>O, <sup>17</sup>O, and <sup>18</sup>O) can be used to distinguish anthropogenic from natural (atmospheric) perchlorate.

#### 5078

#### Interaction of Uranyl with Calcite in the Presence of EDTA

Sophie Rihs, Neil C. Sturchio, Kent Orlandini, Likwan Cheng, Henry Teng, Paul Fenter, and Michael J. Bedzyk

The sorption of uranyl on the calcite surface in the presence of EDTA is studied using batch experiments and synchrotron X-ray standing wave techniques.

#### **5087**

#### Arsenic Occurrence, Mobility, and Retardation in Sandstone and Dolomite Formations of the Fox River Valley, Eastern Wisconsin

Katie Thornburg and Nita Sahai

Oxidative dissolution of the disseminated arsenic-rich  ${\rm FeS}_2$  grains and nodules is sufficient to explain the elevated arsenic levels observed in eastern Wisconsin groundwater.

#### 5095

### In Vivo Synchrotron Study of Thallium Speciation and Compartmentation in *Iberis intermedia*

Kirk G. Scheckel, Enzo Lombi, Steven A. Rock, and Mike J. McLaughlin  $\mu\text{-XANES}$  and  $\mu\text{-XRF}$  in vivo investigations show that significant thallium uptake by *Iberis intermedia* is localized within the vascular network of leaves as aqueous TI(I).

#### 5101

#### Macroscopic and Microscopic Observations of Particle-Facilitated Mercury Transport from New Idria and Sulphur Bank Mercury Mine Tailings

Gregory V. Lowry, Samuel Shaw, Christopher S. Kim, James J. Rytuba, and Gordon E. Brown, Jr.

Mechanisms of mercury release from mine wastes, speciation of released particle-bound mercury, and effect of calcinations on mercury release processes are investigated.

#### 5112

# Potential Role of Chlorination Pathways in PCDD/F Formation in a Municipal Waste Incinerator

Jae-Yong Ryu, James A. Mulholland, James E. Dunn, Fukuya lino, and Brian K. Gullett

The role of chlorination reactions in polychlorinated dibenzo- p-dioxin and dibenzofuran formation in a municipal waste incinerator is assessed on the basis of isomer distributions.

### **Environmental Modeling**

5120

Geostatistical Approach for Assessing Soil Volumes Requiring Remediation: Validation Using Lead-Polluted Soils Underlying a Former Smelting Works

Helene Demougeot-Renard and Chantal De Fouquet

A geostatistical approach for assessing soil volumes requiring remediation is validated with the real remediated volume of a former smelting works.

### **Environmental Measurements Methods**

#### **5127**

Toxicity Characterization of Complex Mixtures Using Biological and Chemical Analysis in Preparation for Assessment of Mixture Similarity

Leslie Cizmas, Thomas J. McDonald, Tracie D. Phillips, Annika M. Gillespie, Rebecca A. Lingenfelter, Leon F. Kubena, Timothy D. Phillips, and Kirby C. Donnelly

Mixture similarity may be assessed using an integrated protocol that includes chemical fractionation and analysis as well as biological characterization of the mixtures.

#### 5134

Azo Dye Method for Mapping Relative Sediment Enzyme Activity in Situ at Precise Spatial Locations

Nicola J. Rogers and Simon C. Apte

A novel probe to map relative sediment enzyme activity in situ at high spatial resolution is described.

#### 5141

Compensation of the Exhaust Gas Transport Dynamics for Accurate Instantaneous Emission Measurements

Delia Ajtay and Martin Weilenmann

Exhaust gas transport systems for typical chassis dynamometer test equipment are modeled to compensate for the variable time delay and convolution of the transport.

### **Remediation and Control Technologies**

#### **5149**

Efficient, Near-Complete Removal of DNAPL from Three-Dimensional, Heterogeneous Porous Media Using a Novel Combination of Treatment Technologies

D. N. Johnson, J. A. Pedit, and C. T. Miller

A promising treatment technology based on surfactant- and gravity-induced mobilization, dense brine containment and collection, and a vapor-phase extraction polishing step is tested.

#### 5157

Chloride Effect on TNT Degradation by Zerovalent Iron or Zinc during Water Treatment

Rafael Hernandez, Mark Zappi, and Chiang-Hai Kuo

Adding chloride, a pitting corrosion promoter, into TNT-contaminated water significantly accelerates the rate of TNT reaction with zerovalent iron or zinc.

#### 5164

Laboratory Assessment of the Mobility of Nanomaterials in Porous Media

Hélène F. Lecoanet, Jean-Yves Bottero, and Mark R. Wiesner

Mobility is evaluated for eight particulate products of nanochemistry. Contrary to assertions that nanomaterials present monolithic environmental risks, these nanomaterials exhibit widely differing transport behaviors.

#### 5170

Potential Remediation of Waters Contaminated with Cr(III), Cu, and Zn by Sorption on the Organic Polymeric Fraction of Olive Mill Wastewater (Polymerin) and Its Derivatives

Renato Capasso, Massimo Pigna, Antonio De Martino, Marianna Pucci, Filomena Sannino, and Antonio Violante

Sorption of mixtures of Cr(III), Cu, and Zn on the humic-acidlike fraction (polymerin) of olive-mill wastewater and some of its derivatives.

#### 5177

Removal of Estrogenic Activity and Formation of Oxidation Products during Ozonation of 17 $\alpha$ -Ethinylestradiol

Marc M. Huber, Thomas A. Ternes, and Urs von Gunten

Estrogenic activity caused by  $17\alpha$ -ethinylestradiol is reduced during ozonation because of the fast oxidation of the parent compound and the formation of inactive oxidation products.

#### 5187

Enhanced Bromate Control during Ozonation: The Chlorine–Ammonia Process

Marc-Olivier Buffle, Sonja Galli, and Urs von Gunten

A mechanistic investigation of the chlorine–ammonia process shows its strong potential to solve the bromate problem during drinking-water ozonation.

#### 5196

Formation of Polychlorinated Dibenzo-p-dioxins/Dibenzofurans from Soot of Benzene and o-Dichlorobenzene Combustion

R. Addink and E. R. Altwicker

Both benzene and o-dichlorobenzene soots produce PCDD/F after  $\text{CuCl}_2$  is added to the reaction; this finding suggests that PCDD/F formation needs a metal chloride.

#### 5201

Mechanisms of Strontium and Uranium Removal from High-Level Radioactive Waste Simulant Solutions by the Sorbent Monosodium Titanate

M. C. Duff, D. B. Hunter, D. T. Hobbs, S. D. Fink, Z. Dai, and J. P. Bradley Mechanisms of uranium(VI) and strontium uptake by the sorbent monosodium titanate in highly caustic radioactive waste simulant solutions are presented.

#### 5208

Congener-Specific Dechlorination of Dissolved PCBs by Microscale and Nanoscale Zerovalent Iron in a Water/ Methanol Solution

Gregory V. Lowry and Kathleen M. Johnson

Dechlorination rates and the resulting dechlorination products afforded by unmodified nanoscale and by palladized microscale zerovalent iron are measured for select PCB congeners.

#### 5217

Formation of Dioxins in the Catalytic Combustion of Chlorobenzene and a Micropollutant-like Mixture on Pt/y-Al.O.

Vincent De Jong, Mariusz K. Cieplik, and Robert Louw

Formation of PCBs, PCDDs, and PCDFs as intermediates/side products from the model compound and synthetic mixture is reported; mechanisms and consequences are discussed.

#### 5224

Significance of Iron(II, III) Hydroxycarbonate Green Rust in Arsenic Remediation Using Zerovalent Iron in Laboratory Column Tests

Chunming Su and Robert W. Puls

Iron(II, III) hydroxycarbonate green rust is a predominant zerovalent iron corrosion product, a sorbent for arsenic, and an oxidizing agent for arsenite in laboratory column tests.

#### 5232

#### Electrochemical Inactivation of Triclosan with Boron-Doped Diamond-Film Electrodes

Jiankang Wang and James Farrell

Although the byproducts of triclosan oxidation become progressively less reactive with increasing electrolysis time, triclosan can be completely oxidized to  $\mathrm{CO}_2$  above 2 mA/cm².

#### 5238

# Peroxidase-Catalyzed Coupling of Phenol in the Presence of Model Inorganic and Organic Solid Phases

Qingguo Huang and Walter J. Weber, Jr.

Model solids influence peroxidase-catalyzed phenol coupling by mitigation of enzyme inactivation, by participation in cross-coupling, or by a combination of these two activities.

#### 5246

# Degradation of *tert*-Butyl Alcohol in Dilute Aqueous Solution by an $O_3/UV$ Process

Temesgen Garoma and Mirat D. Gurol

TBA is oxidized rapidly with acetone, hydroxy-*iso*-butyraldehyde, and formaldehyde as primary intermediates; upon further oxidation, acetic, formic, pyruvic, and oxalic acids and pyruvaldehyde are generated.

Supporting Information is available free of charge via the Internet at http://pubs.acs.org.

### **Sustainability Engineering and Green Chemistry**

#### **5253**

Chemical Structure of Arsenic and Chromium in CCA-Treated Wood: Implications of Environmental Weathering

Peter S. Nico, Scott E. Fendorf, Yvette W. Lowney, Stewart E. Holm, and Michael V. Ruby

The oxidation state and chemical structure of arsenic and chromium in CCA-treated wood were investigated with X-ray absorption spectroscopy.

### **Correspondence and Rebuttal**

#### 526

Comment on "Environmental Assessment of Used Oil Management Methods"

Alan Gressel

#### 5262

Response to Comment on "Environmental Assessment of Used Oil Management Methods"

Bob Boughton and Arpad Horvath

#### 5263

Comment on "A Polymer Membrane Containing Fe<sup>0</sup> as a Contaminant Barrier"

Craig H. Benson and Tuncer B. Edil

#### 5264

Response to Comment on "A Polymer Membrane Containing Fe<sup>0</sup> as a Contaminant Barrier"

T. Shimotori, W. A. Arnold, E. E. Nuxoll, and E. L. Cussler

