

March 15, 2004

# ENVIRONMENTAL Science & Technology

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Atmospheric Emissions of  
**PBDEs** and other  
**POPs** during a Major  
Combustion Event

Controversy Clouds Atrazine Studies

Quantitative Determination of  
Fluorotelomer Sulfonates in Groundwater

PUBLISHED BY  
THE AMERICAN  
CHEMICAL SOCIETY



1675

**Congener-Specific Composition of Polychlorinated Naphthalenes, Coplanar PCBs, Dibenzo-*p*-dioxins, and Dibenzofurans in the Halowax Series**

Yukio Noma, Takashi Yamamoto, and Shin-Ichi Sakai

Congener-specific compositions and dioxin-like toxicities of polychlorinated naphthalenes, coplanar PCBs, dibenzo-*p*-dioxins, and dibenzofurans were determined in all seven Halowax preparations.

1681

**Atmospheric Emissions of Polybrominated Diphenyl Ethers and Other Persistent Organic Pollutants during a Major Anthropogenic Combustion Event**

N. J. Farrar, K. E. C. Smith, R. G. M. Lee, G. O. Thomas, A. J. Sweetman, and K. C. Jones

Data are presented to illustrate the consequences of episodic combustion on the air concentrations of polybrominated diphenyl ethers, polynuclear aromatic hydrocarbons, and polychlorinated biphenyls within the United Kingdom.

1686

**Concentration and Distribution of Platinum Group Elements (Pt, Pd, Rh) in Airborne Particulate Matter in Frankfurt am Main, Germany**

Fathi Zereini, Friedrich Alt, Jürge Messerschmidt, Alex von Bohlen, Karlheinz Liebl, and Wilhelm Püttmann

Results of concentrations and distribution of platinum group elements in airborne particulate matter in urban and nonurban areas in Germany are presented.

**Environmental Processes**

■ 1693

**Vapor Pressures of the Fluorinated Telomer Alcohols—Limitations of Estimation Methods**

Naomi L. Stock, David A. Ellis, Lisa Deleebeeck, Derek C. G. Muir, and Scott A. Mabury

A comparison of measured vapor pressures of FTOHs with estimated values indicates that some estimation models may not account for the unique geometry of fluorinated chemicals.

1700

**X-ray Absorption Spectroscopic Evidence for the Formation of Pb(II) Inner-Sphere Adsorption Complexes and Precipitates at the Calcite–Water Interface**

Ashaki A. Rouff, Evert J. Elzinga, Richard J. Reeder, and Nicholas S. Fisher

Pb(II) sorption products in pH 8.3 calcite–water suspensions are characterized as a function of metal concentration by X-ray absorption spectroscopy.

1708

**Understanding the Role of Iron Chlorides in the De Novo Synthesis of Polychlorinated Dibenzo-*p*-dioxins/Dibenzofurans**

Shawn P. Ryan and Elmar R. Altwicker

The formation of PCDD/F on mixtures containing iron chlorides is reported, and mechanistic implications relating to the de novo synthesis are discussed.

■ 1718

**Modeling the Kinetics of the Competitive Adsorption and Desorption of Glyphosate and Phosphate on Goethite and Gibbsite and in Soils**

Anne Louise Gimsing, Ole K. Borggaard, and Peter Sestoft

Kinetic models to describe the competition between glyphosate and phosphate for adsorption sites on goethite and gibbsite and in soils are described and evaluated.

1723

▶ **A Multibiomarker Approach to Environmental Assessment**

Tamara S. Galloway, Rebecca J. Brown, Mark A. Browne, Awantha Dissanayake, David Lowe, Malcolm B. Jones, and Michael H. Depledge

Ecological relevance has guided the choice of organisms and biomarkers in this multibiomarker environmental assessment of a contaminated estuary in southern England.

1732

**Soot Deposition in the Great Lakes: Implications for Semi-Volatile Hydrophobic Organic Pollutant Deposition**

David R. Buckley, Karl J. Rockne, An Li, and William J. Mills

Soot deposition flux and total mass loading are determined for all five Great Lakes and correlate with PAH deposition in Lake Michigan.

1740

**Effect of Root-Derived Substrates on the Expression of *nah-lux* Genes in *Pseudomonas fluorescens* HK44: Implications for PAH Biodegradation in the Rhizosphere**

Roopa Kamath, Jerald L. Schnoor, and Pedro J. J. Alvarez

Root extracts from various plants were screened for their ability to influence naphthalene dioxygenase expression and enhance microbial degradation of PAHs in the rhizosphere.

■ 1746

**Nonbiological Removal of *cis*-Dichloroethylene and 1,1-Dichloroethylene in Aquifer Sediment Containing Magnetite**

Mark L. Ferrey, Richard T. Wilkin, Robert G. Ford, and John T. Wilson

Long-term microcosm studies demonstrate that nonbiological transformation of *cis*-dichloroethylene is responsible for observed contaminant attenuation in groundwater at a Superfund site in Minnesota.

1753

**Production of Macromolecular Chloramines by Chlorine-Transfer Reactions**

Mary Bedner, William A. MacCrehan, and George R. Helz

During maturation of residual chlorine in wastewater, macromolecular organic chloramines trap significant amounts of disinfectant in forms that are feebly reactive and probably germicidally ineffective.

1759

**Source Strengths for Indoor Human Activities that Resuspend Particulate Matter**

Andrea R. Ferro, Royal J. Kopperud, and Lynn M. Hildemann

Normal human activities in a residence effectively resuspend particulate matter with source strengths ranging from 0.03 to 0.5 mg/min for PM<sub>2.5</sub> and from 0.1 to 1.4 mg/min for PM<sub>5</sub>.

1765

**Perrhenate Uptake by Iron and Aluminum Oxyhydroxides: An Analogue for Pertechnetate Incorporation in Hanford Waste Tank Sludges**

Bradley Wakoff and Kathryn L. Nagy

Aging of iron and aluminum oxyhydroxides in simulated Hanford waste tank sludges results in irreversible uptake of small amounts of perrhenate, an analogue for pertechnetate.

1772

**A Theoretical Study of the Oxidation of Hg<sup>0</sup> to HgBr<sub>2</sub> in the Troposphere**

M. E. Goodsite, J. M. C. Plane, and H. Skov

Theoretical calculations show that the atmospheric lifetime of elemental mercury is largely controlled by recombination with bromine atoms and the thermal stability of HgBr.



1777

### **Bacterial Adhesion and Transport in Porous Media: Role of the Secondary Energy Minimum**

Jeremy A. Redman, Sharon L. Walker, and Menachem Elimelech

Secondary energy minimum plays an important role in bacterial adhesion and transport in porous media as shown by a radial stagnation point flow system.

1786

### **Assessing the Bioavailability of PAHs in Field-Contaminated Sediment Using XAD-2 Assisted Desorption**

Li Lei, Makram T. Suidan, Amid P. Khodadoust, and Henry H. Tabak

An XAD-2 assisted desorption assay was found promising in assessing the bioavailability of polycyclic aromatic hydrocarbons in an aged field-contaminated sediment.

1794

### **Coupling Speciation and Isotope Dilution Techniques To Study Arsenic Mobilization in the Environment**

Rebecca E. Hamon, Enzo Lombi, Paolo Fortunati, Annette L. Nolan, and Mike J. McLaughlin

Different mechanisms controlling arsenic mobility in the environment are identified using a coupled isotopic dilution HPLC-ICP-MS procedure.

## **Environmental Modeling**

■ 1799

### **Estimating Exposure to Chemical Contaminants in Drinking Water**

Eunyoung Kim, John C. Little, and Nancy Chiu

An exposure model for chemical contaminants in household drinking water is developed and subjected to an extensive sensitivity and uncertainty analysis.

1807

### **Applying the Nernst Equation To Simulate Redox Potential Variations for Biological Nitrification and Denitrification Processes**

Cheng-Nan Chang, Hong-Bang Cheng, and Allen C. Chao

Several modified Nernst equations based on the real stoichiometric relationship are developed to simulate the redox potential variations during biological nitrogen removal.

■ 1813

### **Modified Polytopic Vector Analysis To Identify and Quantify a Dioxin Dechlorination Signature in Sediments. 1. Theory**

Noémi Barabás, Peter Adriaens, and Pierre Goovaerts

The ability of a modified PVA procedure to reproduce the dechlorination pattern and its variability contribution depends on the actual contribution of dechlorination to variability.

1821

### **Modified Polytopic Vector Analysis To Identify and Quantify a Dioxin Dechlorination Signature in Sediments. 2. Application to the Passaic River**

Noémi Barabás, Pierre Goovaerts, and Peter Adriaens

Applied to 351 samples, the approach yields opportunities for hypothesis testing whereby ultimate decisions must be made using a combination of different sources of evidence.

## **Environmental Measurements Methods**

1828

### **Quantitative Determination of Fluorotelomer Sulfonates in Groundwater by LC MS/MS**

Melissa M. Schultz, Douglas F. Barofsky, and Jennifer A. Field

Fluorotelomer sulfonates are quantitated in AFFF-contaminated groundwater at U.S. military bases; however, fluoroalkylthio-amido sulfonates are the main anionic fluorosurfactants identified in the fluorotelomer-based AFFF.

1836

### **Quantifying Hazardous Species in Particulate Matter Derived from Fossil-Fuel Combustion**

Frank E. Huggins, Gerald P. Huffman, William P. Linak, and C. Andrew Miller

The combination of X-ray absorption near-edge structure spectroscopy and leaching procedures is used to identify and quantify toxic species in fossil-fuel-derived particulate matter and to indicate their potential bioavailability.

1843

### **Formation of Cu(I) in Estuarine and Marine Waters: Application of a New Solid-Phase Extraction Method to Measure Cu(I)**

Diane Buerge-Weirich and Barbara Sulzberger

Cu(I), enriched as a bathocuproine complex on a hydrophobic polymer column, is analyzed with graphite-furnace absorption spectroscopy and has a detection limit of  $<1 \times 10^{-9}$  M.

1849

### **Estimation of Membrane Diffusion Coefficients and Equilibration Times for Low-Density Polyethylene Passive Diffusion Samplers**

Craig E. Divine and John E. McCray

Membrane diffusion coefficients are measured for LDPE passive diffusion samplers, and these results are used to evaluate sampler equilibration and performance with analytical and numerical models.

## **Remediation and Control Technologies**

1858

### **Microbial Removal of Ionic Mercury in a Three-Phase Fluidized Bed Reactor**

W.-D. Deckwer, F. U. Becker, S. Ledakowicz, and I. Wagner-Döbler

Microbial mercury removal from waste streams was demonstrated in a three-phase fluidized bed with volatilization of the produced elemental mercury followed by its absorptive capture.

■ 1866

### **Effects of Iron Purity and Groundwater Characteristics on Rates and Products in the Degradation of Carbon Tetrachloride by Iron Metal**

María L. Támara and Elizabeth C. Butler

This study reports the effects of iron purity and groundwater characteristics on the rates and products of carbon tetrachloride transformation by zerovalent iron metal.

1877

### **Microcosm Studies for Neutralization of Hypolimnetic Acid Mine Pit Lake Water (pH 2.6)**

R. Frömmichen, K. Wendt-Potthoff, K. Friese, and R. Fischer

Elevated neutralization rates for acid mine pit lake microcosms treated with Carbokalk and wheat straw lead to a neutralization prognosis for field-scale mesocosm studies.

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

► This issue contains a news story about this research.