

July 1, 2005

# ENVIRONMENTAL Science & Technology

<http://pubs.acs.org/est>

## Hexabromocyclododecane **CHALLENGES Scientists and Regulators**

Life Cycle Approaches to  
Sustainable Consumption

Management of Tropospheric Ozone  
by Reducing Methane Emissions

PUBLISHED BY  
THE AMERICAN  
CHEMICAL SOCIETY

## Critical Review

4673

**Life Cycle Approaches to Sustainable Consumption: A Critical Review**

Edgar G. Hertwich

The review of LCA and IOA in sustainable consumption policies indicates the need for more strategic analyses exploring the decision options of policy makers.

## Policy Analysis

■ 4685

**Management of Tropospheric Ozone by Reducing Methane Emissions**

J. Jason West and Arlene M. Fiore

The reduction of methane emissions to decrease global background ozone concentrations is evaluated for air quality management.

■ 4692

**Inter-zonal Tradable Discharge Permit System to Control Water Pollution in Tianjin, China**

Hongbin Cao and Saburo Ikeda

An inter-zone TDP system is proposed, and its cost efficiency and environmental effectiveness for controlling water pollution in Tianjin, China, are analyzed.

## Characterization of Natural and Affected Environments

4700

**Spatial and Temporal Distribution of Polycyclic Aromatic Hydrocarbons in Sediments from Michigan Inland Lakes**

Kurunthachalam Kannan, Boris Johnson-Restrepo, Sharon S. Yohn, John P. Giesy, and David T. Long

Profiles of PAHs in sediment cores collected from 11 Michigan inland lakes are examined to evaluate spatial and temporal trends of contamination.

4707

**Biogeographic Provinces of Total and Methyl Mercury in Zooplankton and Fish from the Beaufort and Chukchi Seas: Results from the SHEBA Drift**

G. A. Stern and R. W. Macdonald

Enrichment of total and methyl mercury concentrations in zooplankton and Arctic cod are associated with oceanographic domains and fronts and, to a lesser extent, mercury depletion events.

4714

**Organochlorine Contaminants in Human Adipose Tissues from China: Mass Balance Approach for Estimating Historical, Chinese Exposure to DDTs**

Haruhiko Nakata, Tetsuya Nasu, Shin-Ichi Abe, Takeshi Kitano, Qiyuan Fan, Weihua Li, and Xucheng Ding

Approximately 80% of DDTs deposited in adipose tissues from China may have been accumulated before the 1990s.

4721

**Environmental and Human Impact of an Old-Timer Incinerator in Terms of Dioxin and PCB Level: A Case Study**

Catherine Pirard, Gauthier Eppe, Anne-Cécile Massart, Sébastien Fierens, Edwin De Pauw, and Jean-François Focant

Notices to *ES&T* authors

1. We are pleased to inaugurate a new subject heading, **Ecotoxicology and Human Environmental Health**, in recognition of the emerging importance of this field and the increasing number of *ES&T* papers being submitted. Look for it soon.
2. Submitted manuscripts must now include email addresses for all coauthors, in addition to full contact information for the corresponding author. Please also provide a list of at least four suggested reviewers and their contact information (email addresses are preferred).
3. Effective now, 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.

The impact of an old incinerator on the surrounding environment and human beings is evaluated.

■ 4729

**Detailed Study of Factors Controlling Atmospheric Concentrations of PCNs**

Robert G. M. Lee, Gareth O. Thomas, and Kevin C. Jones

Atmospheric concentrations of polychlorinated naphthalenes are measured at three sites in the British Isles; a detailed analysis of the factors affecting concentrations is performed.

■ 4739

**Air-Surface Exchange of Gaseous Mercury over a Mixed Sawgrass-Cattail Stand within the Florida Everglades**

Frank J. Marsik, Gerald J. Keeler, Steve E. Lindberg, and Hong Zhang

Although current techniques can adequately quantify gaseous elemental mercury air-surface exchange, measurement uncertainties preclude a more complete understanding of some important exchange processes.

4747

**Sources of Methylmercury to a Wetland-Dominated Lake in Northern Wisconsin**

C. J. Watras, K. A. Morrison, A. Kent, N. Price, O. Regnell, C. Eckley, H. Hintelmann, and T. Hubacher

Studies of a Wisconsin lake challenge the popular wisdom that wetlands are a dominant source of methylmercury; alternative explanations for the correlation between wetland runoff and waterborne methylmercury are offered.

■ 4759

**Limited Temporal Variability of Arsenic Concentrations in 20 Wells Monitored for 3 Years in Araihaazar, Bangladesh**

Z. Cheng, A. van Geen, A. A. Seddique, and K. M. Ahmed

Only limited arsenic variability is found in most monitored tube wells in Bangladesh, with seasonal fluctuations and long-term increases in a few shallow wells.

4767

**Summertime Ambient Formaldehyde in Five U.S. Metropolitan Areas: Nashville, Atlanta, Houston, Philadelphia, and Tampa**

Purnendu K. Dasgupta, Jianzhong Li, Genfa Zhang, Winston T. Luke, William A. McClenny, Jochen Stutz, and Alan Fried

- Supporting information is available free at <http://pubs.acs.org/est>.
- ▶ This issue contains a news story about this research.

Agreement among disparate instruments measuring urban formaldehyde indicates that these measurements can be made reliably and accurately; this data set can serve as a benchmark.

#### ■ 4784

##### **PCDD/Fs in Norwegian and U.K. Soils: Implications for Sources and Environmental Cycling**

Ashraf Hassanin, Robert G. M. Lee, Eiliv Steinnes, and Kevin C. Jones  
PCDD/Fs are fractionated latitudinally in soils but do not exhibit the same air-soil "hopping" behavior as other POPs.

### **Environmental Processes**

#### 4793

##### **Organic and Inorganic Aerosol Below-Cloud Scavenging by Suburban New Jersey Precipitation**

Steven F. Maria and Lynn M. Russell

Measurements during rain events provide chemical and physical aerosol data from which boundary-layer below-cloud scavenging coefficients are derived and their relationship to chemical composition determined.

#### ■ 4801

##### **Trophodynamic Behavior of 4-Nonylphenol and Nonylphenol Polyethoxylate in a Marine Aquatic Food Web from Bohai Bay, North China: Comparison to DDTs**

Jianying Hu, Fen Jin, Yi Wan, Min Yang, Lihui An, Wei An, and Shu Tao

The trophic transfer of 4-nonylphenol and nonylphenol polyethoxylate were determined in 14 marine species.

#### 4808

##### **Spatial Distribution and Speciation of Lead around Corroding Bullets in a Shooting Range Soil Studied by Micro-X-ray Fluorescence and Absorption Spectroscopy**

Delphine Vantelon, Antonio Lanzirrotti, Andreas C. Scheinost, and Ruben Kretzschmar

Analyses of corroding lead bullets in soil by micro-XANES spectroscopy show initial formation of litharge and transformation to hydrocerussite and cerussite in the weathering crusts.

#### 4816

##### **Evaluation of Density Functional Theory Methods for Studying Chemisorption of Arsenite on Ferric Hydroxides**

Nianliu Zhang, Paul Blowers, and James Farrell

Several density functional theory methods are used to determine binding modes and binding energies of arsenite on ferric hydroxide complexes.

#### 4823

##### **Products of Ozone-Initiated Chemistry in a Simulated Aircraft Environment**

Armin Wisthaler, Gyöngyi Tamás, David P. Wyon, Peter Strøm-Tejsten, David Space, Jonathan Beauchamp, Armin Hansel, Tilmann D. Märk, and Charles J. Weschler

Ozone reacts with surfaces inside a simulated aircraft cabin to produce a mixture of oxidation products, including saturated and unsaturated aldehydes as well as squalene oxidation products.

#### 4833

##### **Approaches for Establishing Predicted-No-Effect Concentrations for Population-Level Ecological Risk Assessment in the Context of Chemical Substances Management**

Bin-le Lin, Akihiro Tokai, and Junko Nakanishi

Two approaches are given for determining predicted-no-effect concentrations for use in population-level ecological risk assessment in the context of chemical substances management.

#### 4841

##### **Bioreduction of Uranium in a Contaminated Soil Column**

Baohua Gu, Wei-Min Wu, Matthew A. Ginder-Vogel, Hui Yan, Matthew W. Fields, Jizhong Zhou, Scott Fendorf, Craig S. Criddle, and Philip M. Jardine

Oxidized forms of U(VI) can be reduced to relatively insoluble U(IV) by recirculation of groundwater amended electron donors in the presence of competent microbial populations.

#### 4848

##### **Stable Isotope Evidence for Biodegradation of Chlorinated Ethenes at a Fractured Bedrock Site**

Michelle M. G. Chartrand, Penny L. Morrill, Georges Lacrampe-Couloume, and Barbara Sherwood Lollar

Stable carbon isotope measurements are used to quantify biodegradation of chlorinated ethenes at a TCE-contaminated fractured bedrock site with variable groundwater hydraulic gradients.

#### 4857

##### **Surface-Mediated Formation of Polybrominated Dibenzo-p-dioxins and Dibenzofurans from the High-Temperature Pyrolysis of 2-Bromophenol on a CuO/Silica Surface**

Catherine S. Evans and Barry Dellinger

The role of a CuO/silica surface in mediating the formation of PBDDs and PBDFs from 2-bromophenol is determined for pyrolytic, post-flame-combustion conditions.

#### ■ 4864

##### **Relation of Organic Contaminant Equilibrium Sorption and Kinetic Uptake in Plants**

Hui Li, Guangyao Sheng, Cary T. Chiou, and Ouyong Xu

Plant uptake of lipophilic organic contaminants from water increases with exposure time, approaching the limit defined by equilibrium sorption.

#### 4871

##### **Dissolution Kinetics of Synthetic Zeolite NaP1 and Its Implication to Zeolite Treatment of Contaminated Waters**

Jordi Cama, Carles Ayora, Xavier Querol, and Jiwchar Ganor

The dissolution rate of a synthetic zeolite used for the treatment of contaminated waters is relatively fast and pH-dependent.

#### 4878

##### **Competitive Sorption between 17 $\alpha$ -Ethinyl Estradiol and Naphthalene/Phenanthrene by Sediments**

Zhiqiang Yu and Weilin Huang

The competitive effects of EE2 on naphthalene sorption and of phenanthrene on EE2 sorption are observed, but little effect is found.

#### ■ 4886

##### **Analysis of Copper Binding in the Ternary System Cu<sup>2+</sup>/Humic Acid/Goethite at Neutral to Acidic pH**

Takumi Saito, Luuk K. Koopal, Shinya Nagasaki, and Satoru Tanaka

Adsorption of humic acid on goethite enhances the binding of copper to the humic acid/goethite complex; possible mechanisms for this enhancement are proposed.

#### 4894

##### **Enrichment of Excess <sup>210</sup>Po in Anoxic Ponds**

Guebuem Kim, Su-Jin Kim, Koh Harada, Michael K. Schultz, and William C. Burnett

Polonium-210, a naturally occurring radionuclide in the uranium decay chain, is enriched in anoxic ponds as a result of reduction of sedimentary Fe/Mn oxides.

■ Supporting information is available free at <http://pubs.acs.org/est>.

4900

**Kinetic Characterization of *Methanobacterium bryantii* M.o.H.**

Fatih Karadagli and Bruce E. Rittmann

Monod kinetic constants are described for a methanogenic microorganism that uses only H<sub>2</sub> as its electron donor.

■ 4906

**Adsorption of Aqueous Uranyl Complexes onto *Bacillus subtilis* Cells**

Drew Gorman-Lewis, Patricia E. Elias, and Jeremy B. Fein

U(VI) adsorption onto *Bacillus subtilis* cells is measured in the presence and absence of dissolved CO<sub>2</sub> and in the presence of dissolved CO<sub>2</sub> and Ca.

4913

**Characterizing and Quantifying Controls on Arsenic Solubility over a pH Range of 1–11 in a Uranium Mill-Scale Experiment**

Brett J. Moldovan and M. Jim Hendry

Thermodynamic controls on the solubility of arsenic from pH 1 to 11 were assessed using a mill-scale experiment.

■ 4921

**Oxidative Dissolution of Chromium(III) Hydroxide at pH 9, 3, and 2 with Product Inhibition at pH 2**

Giehyeon Lee and Janet G. Hering

Sodium hypochlorite promotes the dissolution of chromium(III) hydroxide strongly at pH 9 and to a lesser extent at pH 3 and 2, with product inhibition observed at pH 2.

## Environmental Modeling

■ 4929

**Estimation of Fugitive Lead Emission Rates from Secondary Lead Facilities using Hierarchical Bayesian Models**

Amit Goyal, Mitchell J. Small, Katherine von Stackelberg, Dmitriy Burmistrov, and Nancy Jones

A methodology is presented and implemented at three sites; this study demonstrates how information from multiple sites can be combined and considered simultaneously.

■ 4938

**Deconvolution and Quantification of Hydrocarbon-like and Oxygenated Organic Aerosols Based on Aerosol Mass Spectrometry**

Qi Zhang, M. Rami Alfarra, Douglas R. Worsnop, James D. Allan, Hugh Coe, Manjula R. Canagaratna, and Jose L. Jimenez

Organic source apportionment can be performed on the basis of total particle mass rather than on the basis of organic tracer compounds.

■ 4953

**Sources of Fine Particles in a Rural Midwestern U.S. Area**

Eugene Kim, Philip K. Hopke, Donna M. Kenski, and Michael Koerber

Positive matrix factorization is applied to an ambient PM<sub>2.5</sub> compositional data set of 24-h integrated samples collected at a monitoring site in Bondville, Ill.

4961

**Quantitative Structure–Activity Relationship Models for Prediction of the Toxicity of Polybrominated Diphenyl Ether Congeners**

Yawei Wang, Huanxiang Liu, Chunyan Zhao, Hanxia Liu, Zongwei Cai, and Guibin Jiang

Factors influencing PBDEs' binding affinities to AhR are studied, and the pI values of PBDEs for which experimental data are unavailable are predicted with QSAR models.

## Environmental Measurements Methods

4967

**New Real-Time Technique to Measure the Size Distribution of Water-Insoluble Aerosols**

Roby Greenwald, Michael H. Bergin, Christian M. Carrico, and Don Grant

A sampling apparatus is developed that entrains atmospheric aerosols in a liquid stream and uses an optical technique to size and count particles remaining in the solid phase.

4974

**Determination of MeHg in Environmental Sample Matrices Using Hg–Thiourea Complex Ion Chromatography with On-line Cold Vapor Generation and Atomic Fluorescence Spectrometric Detection**

Christopher W. Shade and Robert J. M. Hudson

Mercury speciation analysis by Hg–thiourea complex ion chromatography with CVAFS detection is described and applied to the measurement of MeHg in extracts from environmental reference materials.

■ 4983

**In Situ Assessment of Biodegradation Potential Using Biotraps Amended with <sup>13</sup>C-Labeled Benzene or Toluene**

R. Geyer, A. D. Peacock, A. Miltner, H.-H. Richnow, D. C. White, K. L. Sublette, and M. Kästner

A new tool for qualitative assessment of in situ biodegradation of benzene and toluene under actual aquifer conditions uses biotraps amended with <sup>13</sup>C-labeled benzene or toluene.

■ 4990

**Nitrogen and Carbon Dioxide Adsorption by Soils**

Peter I. Ravikovitch, Bill W. Bogan, and Alexander V. Neimark

A correlation between N<sub>2</sub> and CO<sub>2</sub> adsorption on soils, as related to the characterization of soil organic matter, is presented.

4996

**Development of U.S. EPA Method 527 for the Analysis of Selected Pesticides and Flame Retardants in the UCMR Survey**

Barry V. Pepich, Brahm Prakash, Mark M. Domino, Teri A. Dattilio, David J. Munch, and Ed K. Price

Careful optimization of experimental parameters and sample preservation conditions yields an analytical method for occurrence monitoring of selected pesticides and flame retardants under the unregulated contaminant monitoring rule.

5005

**Simple Immunoassay for Detection of PCBs in Transformer Oil**

Thomas R. Glass, Naoya Ohmura, Yukihiko Taemi, and Takashi Joh

A simple, two-step liquid–liquid extraction that uses acidic dimethyl sulfoxide in conjunction with an immunoassay is demonstrated.

5010

**Optical Oxygen Microrespirometry as a Platform for Environmental Toxicology and Animal Model Studies**

Fiach C. O'Mahony, Ciara O'Donovan, James Hynes, Tom Moore, John Davenport, and Dmitri B. Papkovsky

New methodology for testing physiological responses of small organisms monitors changes in oxygen respiration by fluorescence-based oxygen sensing.

## Remediation and Control Technologies

■ 5015

**Decontamination of Uranium-Contaminated Steel Surfaces by Hydroxycarboxylic Acid with Uranium Recovery**

A. J. Francis, C. J. Dodge, J. A. McDonald, and G. P. Halada

A comprehensive, simple, and safe method is described for decontamination of uranium-contaminated metallic surfaces with citric acid, common soil bacteria, and sunlight.

■ **5022**

**Temperature Effects on the Morphology of Porous Thin Film Composite Nanofiltration Membranes**

Ramesh R. Sharma and Shankararaman Chellam

Raising the feedwater temperature changes nanofiltration membrane morphology by increasing pore sizes and decreasing pore density, thereby reducing contaminant rejection.

**5031**

**Catalytic Oxidation of S(IV) in Seawater Slurries of Activated Carbon**

B. F. Vidal, P. Ollero, F. J. Gutiérrez Ortiz, and R. Arjona

The catalytic oxidation of S(IV) in seawater slurries of activated carbon is first-order with respect to S(IV) and zeroth-order with respect to oxygen.

**5037**

**Wireless Sensors Powered by Microbial Fuel Cells**

Avinash Shantaram, Haluk Beyenal, Raaja Raajan Angathevar Veluchamy, and Zbigniew Lewandowski

Electrical energy generated by microbial fuel cells is stored and used in short bursts of adequate power for commercial electronic components.

**5043**

**SH Radical: The Key Intermediate in Sulfur Transformation during Thermal Processing of Coal**

Jinding Yan, Jianli Yang, and Zhenyu Liu

The SH radical interacts with char to form secondary sulfur compounds, whereas H<sub>2</sub>S and SO<sub>2</sub> play no role in sulfur transformation to the carbon structure.

**5052**

**Fenton-Mediated Oxidation in the Presence and Absence of Oxygen**

Christopher K. Duesterberg, William J. Cooper, and T. David Waite

The presence of oxygen significantly reduces the efficiency of Fenton-mediated degradation of chain-promoting organic compounds, such as formic acid.

**5059**

**4-Nitrophenol Biodegradation in a Sequencing Batch Reactor Operating with Aerobic-Anoxic Cycles**

M. Concetta Tomei and M. Cristina Annesini

The study presents the results of a 4-nitrophenol removal process performed in a lab-scale sequential batch reactor with an integrated aerobic-anoxic cycle.

**5066**

**Phenol Chlorination and Photochlorination in the Presence of Chloride Ions in Homogeneous Aqueous Solution**

Davide Vione, Valter Maurino, Claudio Minero, Paola Calza, and Ezio Pelizzetti

Phenol chlorination is assessed in the presence of dissolved Fe(III), hydrogen peroxide, and chloride—important environmental factors in atmospheric aerosols.

**5076**

**Removal of  $\alpha$ -Picoline,  $\beta$ -Picoline, and  $\gamma$ -Picoline from Synthetic Wastewater Using Low Cost Activated Carbons Derived from Coconut Shell Fibers**

Dinesh Mohan, Kunwar P. Singh, and Deblina Ghosh

Equilibrium and kinetic adsorption studies at different pH, temperatures, particle sizes, and solid-to-liquid ratios are used to evaluate two types of activated carbons for the remediation of  $\alpha$ -,  $\beta$ -, and  $\gamma$ -picolines from water/wastewater.

**5087**

**High-Temperature Sorption of Cesium and Strontium on Dispersed Kaolinite Powders**

Jong-Ik Yoo, Takuya Shinagawa, Joseph P. Wood, William P. Linak, Dawn A. Santoianni, Charles J. King, Yong-Chil Seo, and Jost O. L. Wendt

Sorption is investigated as a means to minimize cesium and strontium emissions during high-temperature processes being developed to isolate and dispose of radiological and mixed wastes.

■ **5095**

**Use of Potassium Formate in Road Winter Deicing Can Reduce Groundwater Deterioration**

Pasi P. Hellstén, Jani M. Salminen, Kirsten S. Jørgensen, and Taina H. Nystén

This field-scale study shows that rapid biodegradation of formate in soil at low temperatures makes potassium formate a promising candidate for sustainable winter road maintenance.

**5101**

**Controlling Formaldehyde Emissions with Boiler Ash**

Jennifer Cowan, Malyuba Abu-Daibes, and Sujit Banerjee

Formaldehyde is stripped from an airstream by fluidized wood ash through initial partitioning to ash moisture, followed by rate-controlling binding to ash solids.

■ Supporting information is available free at <http://pubs.acs.org/est>.