

July 15, 2005

# ENVIRONMENTAL Science & Technology

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

## **Biofiltration *for* Mitigating METHANE Emissions *from* Animal Husbandry**



**Research Priorities for Airborne Particulate  
Matter in the United States**

**Gonadal Development of Larval Male *Xenopus laevis*  
Exposed to Atrazine in Outdoor Microcosms**

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CHEMICAL SOCIETY**

## Policy Analysis

■ 5105

### PM<sub>2.5</sub> of Ambient Origin: Estimates and Exposure Errors Relevant to PM Epidemiology

Qing Yu Meng, Barbara J. Turpin, Andrea Polidori, Jong Hoon Lee, Clifford Weisel, Maria Morandi, Steven Colome, Thomas Stock, Arthur Winer, and Jenfeng (Jim) Zhang

Measuring central-site particulate matter results in underestimates of the ambient PM<sub>2.5</sub> exposure distribution bandwidth and leads to larger uncertainties in relative risk factors for PM<sub>2.5</sub>.

## Characterization of Natural and Affected Environments

5113

### Determination of Steroidal Hormone Profiles along the Jalle d'Eysines River (near Bordeaux, France)

Pierre Labadie and H el ene Budzinski

The fate of steroid hormones in riverine systems appears to be season-dependent, and the natural estrogen estrone is relatively persistent under winter conditions.

■ 5121

### ► Is House Dust the Missing Exposure Pathway for PBDEs? An Analysis of the Urban Fate and Human Exposure to PBDEs

Heather A. Jones-Otazo, John P. Clarke, Miriam L. Diamond, Josephine A. Archbold, Glenn Ferguson, Tom Harner, G. Mark Richardson, John Jake Ryan, and Bryony Wilford

Fate calculations indicate that in Toronto, most PBDEs originate within the city; elevated levels in homes result in house dust being the main exposure pathway.

5131

### Record of Metal Workshops in Peat Deposits: History and Environmental Impact on the Mont Loz ere Massif, France

S. Baron, M. Lavoie, A. Ploquin, J. Carignan, M. Pulido, and J.-L. De Beaulieu

This geochemical study reconstructs the history of regional metallurgical activity and demonstrates the existence of a Celtic tribe known for its experience in silver metallurgical processing.

5141

### Organic Compounds Produced during the Thermal Decomposition of Cotton Fabrics

Julia Molt o, Juan A. Conesa, Rafael Font, and Ignacio Mart ın-Gull on

Potentially hazardous organic compounds produced during the thermal decomposition of cotton fabrics are evaluated to determine whether these fabrics could be used as combustion biomass.

■ 5148

### Deriving Sediment Quality Guidelines from Field-Based Species Sensitivity Distributions

Kenneth M. Y. Leung, Anders Bjorgesjter, John S. Gray, W. K. Li, Gilbert C. S. Lui, Yuan Wang, and Paul K. S. Lam

A novel method uses field-based species sensitivity distributions to derive ecologically relevant sediment quality guidelines for existing chemicals.

5157

### Transport of Chemical and Microbial Compounds from Known Wastewater Discharges: Potential for Use as Indicators of Human Fecal Contamination

## 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.

Susan T. Glassmeyer, Edward T. Furlong, Dana W. Kolpin, Jeffery D. Cahill, Steven D. Zaugg, Stephen L. Werner, Michael T. Meyer, and David D. Kryak

Pharmaceuticals and other household chemicals commonly found in wastewater treatment plant effluents can act as tracers of human wastewater discharge.

5170

### Typical Dioxin Concentrations in Agriculture Soils of Washington State and Potential Sources

David L. Rogowski and William Yake

Agricultural soils in the state of Washington have low levels of dioxins (0.14 ng/kg toxicity equivalents) that do not appear to be directly attributable to known dioxin sources.

5177

### ► Polybrominated Diphenyl Ethers and Polychlorinated Biphenyls in Human Adipose Tissue from New York

Boris Johnson-Restrepo, Kurunthachalam Kannan, David P. Rapaport, and Bruce D. Rodan

Concentrations of PBDEs in human adipose tissue from New York City are similar to or greater than concentrations of PCBs.

## Environmental Processes

■ 5183

### Hexahydro-1,3,5-trinitro-1,3,5-triazine Transformation by Biologically Reduced Ferrihydrite: Evolution of Fe Mineralogy, Surface Area, and Reaction Rates

Aaron G. B. Williams, Kelvin B. Gregory, Gene F. Parkin, and Michelle M. Scherer

Incubation time is an important variable for evaluating and comparing rates of contaminant transformation by biologically reduced iron solids.

5190

### Perchlorate Affects Thyroid Function in Eastern Mosquitofish (*Gambusia holbrooki*) at Environmentally Relevant Concentrations

Carrie M. Bradford, Jacques Rinchar, James A. Carr, and Christopher Theodorakis

Perchlorate affects mosquitofish thyroid histopathology and, to a lesser extent, whole-body thyroxin in a time- and dose-dependent fashion at concentrations as low as 0.1 mg/L.

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

5196

### Three-Dimensional Mapping of Oxygen Distribution in Wastewater Biofilms Using an Automation System and Microelectrodes

Carlos de la Rosa and Tong Yu

Combined oxygen microelectrodes and an automation system are used to map the 3-D oxygen distribution in wastewater biofilms sampled from rotating biological contactors.

5203

### Multiphase Decomposition of Novel Oxygenated Organics in Aqueous and Organic Media

Tamar Moise, Yinon Rudich, Davy Rousse, and Christian George

Kinetic information is provided on the multiphase oxidation of a series of saturated and unsaturated oxygenated compounds by the OH radical and by ozone.

5209

### Environmental Fate of Pharmaceuticals in Water/Sediment Systems

Dirk Löffler, Jörg Römbke, Michael Meller, and Thomas A.ernes

The fates of pharmaceuticals—such as carbamazepine, diazepam, ibuprofen, iopromide, ivermectin, and paracetamol—and a few corresponding human metabolites in water–sediment systems are described.

5219

### Solar Radiation, Relative Humidity, and Soil Water Effects on Metolachlor Volatilization

John H. Prueger, Timothy J. Gish, Laura L. McConnell, Lynn G. Mckee, Jerry L. Hatfield, and William P. Kustas

Metolachlor volatilization is monitored over a five-year period; soil properties, tillage practices, surface residue management, and pesticide formulations are held constant.

5227

### Link between Chemotactic Response to Ni<sup>2+</sup> and its Adsorption onto the *Escherichia coli* Cell Surface

David Borrok, M. Jack Borrok, Jeremy B. Fein, and Laura L. Kiessling

Chemotactic responses to Ni<sup>2+</sup> by *E. coli* are linked to the surface adsorption of Ni<sup>2+</sup>, which can be thermodynamically modeled to predict chemotactic movement.

■ 5234

### Mineralization of Organic Sulfur Delays Recovery from Anthropogenic Acidification

Carl-Magnus Mörh, Peter Torssander, O. Janne Kjønaas, Arne O. Stuanes, Filip Moldan, and Reiner Giesler

Loss of sulfate from the aqueous horizon in a forested catchment is the major contributor of runoff sulfate after experimental reduction of anthropogenic sulfur deposition.

■ 5241

### Comparison of a Chemical and Enzymatic Extraction of Arsenic from Rice and an Assessment of the Arsenic Adsorption from Contaminated Water by Cooked Rice

Amanda H. Ackerman, Patricia A. Creed, Amy N. Parks, Michael W. Fricke, Carol A. Schweigel, John T. Creed, Douglas T. Heitkemper, and Nohora P. Vela

An arsenic-speciation-based exposure assessment is presented for raw rice and rice prepared in contaminated water with both a chemical and an enzymatic extraction approach.

5247

### Calcium-(Organo)aluminum-proton Competition for Adsorption to Tomato Root Cell Walls: Experimental Data and Exchange Model Calculations

Jacqueline W. M. Postma, Willem G. Keltjens, and Willem H. van Riemsdijk

Aluminum displacement of calcium and protons at cell-wall binding sites depends on pH and organic anions and is described with a Gaines–Thomas exchange model.

■ 5255

### Gonadal Development of Larval Male *Xenopus laevis* Exposed to Atrazine in Outdoor Microcosms

Alarik M. Jooste, Louis H. Du Preez, James A. Carr, John P. Giesy, Timothy S. Gross, Ronald J. Kendall, Ernest E. Smith, Glen L. Van Der Kraak, and Keith R. Solomon

Atrazine exposures from 0 to 25 µg/L do not increase incidence of testicular oocytes in *Xenopus* tadpoles; however, numbers of oocytes decrease as frogs mature.

5262

### Electricity Generation from Artificial Wastewater Using an Upflow Microbial Fuel Cell

Zhen He, Shelley D. Minter, and Largus T. Angenent

The upflow microbial fuel cell is a promising wastewater treatment process that can generate electricity and purify wastewater simultaneously for periods >5 months.

5268

### Natural Humics Impact Uranium Bioreduction and Oxidation

Baohua Gu, Hui Yan, Ping Zhou, David B. Watson, Melora Park, and Jonathan Istok

Humic substances enhance the biological reduction of U(VI) under anaerobic conditions and accelerate the oxidation of reduced U(IV)–humic complexes under oxic conditions.

■ 5276

### On-Road Emission Rates of PAH and *n*-Alkane Compounds from Heavy-Duty Diesel Vehicles

Sandip D. Shah, Temitope A. Ogunyoku, J. Wayne Miller, and David R. Cocker III

Per-mile and per-CO<sub>2</sub> emission rates of PAHs and *n*-alkanes are highest for operation simulating congested traffic and lowest for cruising conditions.

5285

### Impact of Vegetation on Sedimentary Organic Matter Composition and Polycyclic Aromatic Hydrocarbon Attenuation

Samuel T. Gregory, Damian Shea, and Elizabeth Guthrie-Nichols

Plant carbon inputs influence the fate of alkylated and non-alkylated PAHs in refinery waste sediment and enhance PAH degradation in labile and refractory sediment fractions.

5293

### Influence of Agricultural Biomass Burning on Aerosol Size Distribution and Dry Deposition in Southeastern Brazil

Gisele O. da Rocha, Andrew G. Allen, and Arnaldo A. Cardoso

Dry deposition fluxes of soluble species increase during winter, which is when sugarcane trash is burned and a large, stationary, dry air mass extends over southern Brazil.

5302

### Reactions of Chlorine Atoms with a Series of Aromatic Hydrocarbons

Lin Wang, Janet Arey, and Roger Atkinson

A relative-rate technique is used to measure rate constants for the reactions of chlorine atoms with naphthalene, methylnaphthalene, and ethylnaphthalene.

■ 5311

### Formation and Dissolution of Single and Mixed Zn and Ni Precipitates in Soil: Evidence from Column Experiments and Extended X-ray Absorption Fine Structure Spectroscopy

Andreas Voegelien and Ruben Kretzschmar

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

Zinc and nickel in soil precipitate into a mixed, layered, double hydroxide that dissolves faster at pH 3.0 than the nickel precipitate formed in the absence of zinc.

**5319**

### **Effect of Humic and Fulvic Acid Concentrations and Ionic Strength on Copper and Lead Binding**

Iso Christl, Axel Metzger, Ilona Heidmann, and Ruben Kretzschmar

Binding isotherms of  $\text{Cu}^{2+}$  and  $\text{Pb}^{2+}$  to humic and fulvic acids are independent of the organic-matter concentration (1–1000 mg/L) and are predicted by the NICA–Donnan model.

**5327**

### **Hierarchical Responses of Soil Invertebrates (Earthworms) to Toxic Metal Stress**

David J. Spurgeon, Huw Ricketts, Claus Svendsen, A. John Morgan, and Peter Kille

Comparison of biological effects of metal exposure demonstrates the sensitivity of low organization effects but a dependence of higher organization effects on species sensitivity.

■ **5335**

### **Photoinduced Oxidation of Antimony(III) in the Presence of Humic Acid**

Johanna Buschmann, Silvio Canonica, and Laura Sigg

Photoinduced oxidation of Sb(III) in the presence of humic acid is most probably caused by excited triplet states and/or phenoxyl radicals.

**5342**

### **Identification of Hydroxylated Polybrominated Diphenyl Ether Metabolites in Blood Plasma from Polybrominated Diphenyl Ether Exposed Rats**

Tina Malmberg, Maria Athanasiadou, Göran Marsh, Ingvar Brandt, and Åke Bergman

Hydroxylated PBDE metabolites are retained in the plasma of rats exposed to PBDEs, similar to hydroxylated PCB metabolites in animals exposed to PCBs.

## **Environmental Modeling**

**5349**

### **Receiver Operating Characteristic Analysis for Environmental Diagnosis. A Potential Application to Endocrine Disruptor Screening: In Vitro Estrogenicity Bioassays**

Olwenn V. Martin, Ka Man Lai, Mark D. Scrimshaw, and John N. Lester

Receiver operating characteristic analysis is applied to in vitro estrogenicity bioassays to characterize their accuracy in terms of both sensitivity and specificity.

**5356**

### **Changes in Motor Vehicle Emissions on Diurnal to Decadal Time Scales and Effects on Atmospheric Composition**

Robert A. Harley, Linsey C. Marr, Jaime K. Lehner, and Sarah N. Giddings

Temporal patterns in emissions from on-road engines are described with California data collected when diesel fuel use grew 3 times faster than gasoline use.

■ **5363**

### **Biochemical Reaction Network Modeling: Predicting Metabolism of Organic Chemical Mixtures**

Arthur N. Mayeno, Raymond S. H. Yang, and Brad Reisfeld

Computational modeling predicts new metabolites and pathway interactions for the metabolism of a mixture of four common volatile organic chemicals.

■ **5372**

### **Modeling Salt-Dependent Proton Binding by Organic Soils with the NICA–Donnan and Stockholm Humic Models**

Jon Petter Gustafsson and Dan Berggren Kleja

The proton binding of solid humic substances is more salt-dependent than that of dissolved humic substances; this has implications for modeling.

## **Environmental Measurements Methods**

**5378**

### **Detection of Herbicide Subclasses by an Optical Multibiosensor Based on an Array of Photosystem II Mutants**

Maria Teresa Giardi, Licia Guzzella, Pierre Euzet, Regis Rouillon, and Dania Esposito

A multibiosensor is developed on the basis of the fluorescence of photosystem II; photosynthetic herbicide subclasses are distinguished with biomediators isolated from mutated organisms.

**5385**

### **Immobilization of Humic Acid in Nanostructured Layer-by-Layer Films for Sensing Applications**

Frank N. Crespilho, Valtencir Zucolotto, José R. Siqueira, Jr., Carlos J. L. Constantino, Francisco C. Nart, and Osvaldo N. Oliveira, Jr.

Humic acids are immobilized in nanostructured layered films in conjunction with cationic polyelectrolytes, which are used as electrochemical sensors for pentachlorophenol.

**5390**

### **Online Volatile Organic Compound Measurements Using a Newly Developed Proton-Transfer Ion-Trap Mass Spectrometry Instrument during New England Air Quality Study—Intercontinental Transport and Chemical Transformation 2004: Performance, Intercomparison, and Compound Identification**

Carsten Warneke, Shuji Kato, Joost A. de Gouw, Paul D. Goldan, William C. Kuster, Min Shao, Edward R. Lovejoy, Ray Fall, and Fred C. Fehsenfeld

A new PIT MS instrument for online VOC measurements is deployed in the field for the first time. The measurements agree well with GC/MS and also improve the identification of VOCs.

**5398**

### **Evaluation of 1047-nm Photoacoustic Instruments and Photoelectric Aerosol Sensors in Source-Sampling of Black Carbon Aerosol and Particle-Bound PAHs from Gasoline and Diesel Powered Vehicles**

W. P. Arnott, B. Zielinska, C. F. Rogers, J. Sagebiel, Kihong Park, Judith Chow, Hans Moosmüller, John G. Watson, K. Kelly, D. Wagner, A. Sarofim, J. Lighty, and G. Palmer

Photoacoustic instruments use compact, efficient, solid-state lasers with direct electronic modulation capabilities and operate at a wavelength of 1047 nm, where gaseous interference is negligible.

**5407**

### **Simple Method for Quantifying Microbiologically Assisted Chloramine Decay in Drinking Water**

Arumugam Sathasivan, Ian Fisher, and George Kastl

A novel method is presented to quantify microbiologically accelerated chloramine decay as a tool to better diagnose and control chloramine residual in drinking-water distribution systems.

■ **5414**

### **Inclusion of Bisphenols by a Self-Assembled Monolayer of Thiolated Calix[6]arene on a Gold Surface**

Tadashi Nakaji-Hirabayashi, Hiroshi Endo, Hideaki Kawasaki, Makoto Gemmei-ide, and Hiromi Kitano

Molecular recognition of bisphenols by a self-assembled monolayer of thiolated calix[6]arene on a gold electrode suggests the possibility of a highly sensitive sensor for endocrine disrupters.

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