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# ENVIRONMENTAL Science & Technology

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Rankin's Grocery

## Leaded-Gasoline ADDITIVES Still Contaminate Groundwater

Linking Observable Stable Isotope Fractionation to Transformation Pathways of Organic Pollutants

Uncertainty in Octanol-Water Partition Coefficient: Implications for Risk Assessment and Remedial Costs

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CHEMICAL SOCIETY

## Critical Reviews

6881

**Extensive Sorption of Organic Compounds to Black Carbon, Coal, and Kerogen in Sediments and Soils: Mechanisms and Consequences for Distribution, Bioaccumulation, and Biodegradation**

Gerard Cornelissen, Örjan Gustafsson, Thomas D. Bucheli, Michiel T. O. Jonker, Albert A. Koelmans, and Paul C. M. van Noort

Sorption to carbonaceous materials can explain high distribution ratios, slow desorption, and limited bioaccumulation/biodegradation.

■ 6896

**A New Concept Linking Observable Stable Isotope Fractionation to Transformation Pathways of Organic Pollutants**

Martin Elsner, Luc Zwank, Daniel Hunkeler, and René P. Schwarzenbach

Bulk compound isotope fractionation of organic pollutants is converted into apparent kinetic isotope effects, which elucidates contaminant degradation pathways and the magnitude and variability of isotopic enrichment factors.

## Policy Analysis

■ 6917

**Uncertainty in Octanol–Water Partition Coefficient: Implications for Risk Assessment and Remedial Costs**

Igor Linkov, Michael R. Ames, Edmund A. C. Crouch, and F. Kyle Satterstrom

A food-chain model for contaminated sediments is used to examine the influence of uncertainty in regulatory-recommended PCB octanol–water partition coefficient ( $K_{ow}$ ) values on risk-based remedial goals and costs.

**Characterization of Natural and Affected Environments**

6923

**Aqueous Stability of Gadolinium in Surface Waters Receiving Sewage Treatment Plant Effluent, Boulder Creek, Colorado**

Philip L. Verplanck, Howard E. Taylor, D. Kirk Nordstrom, and Larry B. Barber

This study of a 14-km reach of a creek dominated by effluent from a sewage treatment plant demonstrates that gadolinium anomalies are persistent, useful tracers of urban wastewater.

■ 6930

**Characterization of Freshwater Natural Aquatic Colloids by Atomic Force Microscopy (AFM)**

J. R. Lead, D. Muirhead, and C. T. Gibson

According to quantification by AFM, natural aquatic colloids have complex structures and form coherent surface films on surfaces.

6937

**Gas-Phase Chemistry of  $\alpha$ -Terpineol with Ozone and OH Radical: Rate Constants and Products**

J. R. Wells

$\alpha$ -Terpineol is a component of cleaning formulations and rapidly reacts with both the OH radical and ozone to form low-molecular-weight, oxygenated organic compounds.

Notices to *ES&T* authors

1. Beginning immediately, *ES&T* will stringently enforce the 7000-word length limit for research manuscripts. Articles are expected to be clear, concise, and comprehensive (not a fragmented story). Manuscripts may exceed the 7000-word limit under highly unusual circumstances, but the length must be justified at submission. Lengthy papers risk being summarily declined. Tables and figures that augment the article but are otherwise unessential to the major themes must be placed in Supporting Information (which is freely accessible on the web). Authors should provide a word count in their cover letter. The count should include all text and references, and 300 words should be added for each figure and table. Large, multipart figures and extensive tables should be counted as 600 words.
2. 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.
3. 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).

6944

**Polychlorinated Biphenyl Concentrations in Adult Chinook Salmon (*Oncorhynchus tshawytscha*) Returning to Coastal and Puget Sound Hatcheries of Washington State**

Brian R. Missildine, Roger J. Peters, Gerardo Chin-Leo, and Douglas Houck

PCB concentrations in adult hatchery chinook salmon from Puget Sound are almost 2.5 $\times$  greater than in adult chinook salmon from hatcheries on the Washington coast.

■ 6952

**Persistent Organic Pollutants in British Columbia Grizzly Bears: Consequence of Divergent Diets**

Jennie R. Christensen, Misty MacDuffee, Robie W. Macdonald, Michael Whitticar, and Peter S. Ross

Shifts in stable isotope profiles along grizzly bear hair reveal two divergent diets and explain contrasting POP patterns in their tissues.

6961

**Combustion Products of Plastics as Indicators for Refuse Burning in the Atmosphere**

Bernd R. T. Simoneit, Patricia M. Medeiros, and Borys M. Didyk

Diethylhexyl phthalate, 1,3,5-triphenylbenzene, and tris(2,4-di-*tert*-butylphenyl)phosphate are found in smoke from burn source tests of plastics and in atmospheric particulate matter; the latter two compounds are proposed as specific tracers for the open burning of plastics.

6971

**Nitration of Benzo[a]pyrene Adsorbed on Coal Fly Ash Particles by Nitrogen Dioxide: Role of Thermal Activation**

Robert L. Kristovich and Prabir K. Dutta

On the basis of GC/MS, DRIFTS, and ESR spectroscopy, a mechanism is proposed for nitration involving intermediates of benzo[a]pyrene radical cations generated on thermally activated aluminosilicate particles.

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

6978

### **Tissue Distribution of Perfluorinated Chemicals in Harbor Seals (*Phoca vitulina*) from the Dutch Wadden Sea**

Kristin Inneke Van de Vijver, Philippe Hoff, Krishna Das, Sophie Brasseur, Walter Van Dongen, Eddy Esmans, Peter Reijnders, Ronny Blust, and Wim De Coen

This paper presents a baseline study on the compound-specific distribution of perfluorinated acids and the occurrence of perfluorobutane sulfonate in harbor seals from Western Europe.

■ 6985

### **Photochemical Mineralization of Dissolved Organic Nitrogen to Ammonium in the Baltic Sea**

Anssi V. Vähätalo and Richard G. Zepp

Photoammonification approximately equals and, on sunny summer days, periodically exceeds the rate of atmospheric deposition of reactive inorganic nitrogen to the northern Baltic Sea.

6993

### **Winter-Time Climatic Control on Dissolved Organic Carbon Export and Surface Water Chemistry in an Adirondack Forested Watershed**

Ji-Hyung Park, Myron J. Mitchell, and Charles T. Driscoll

Snowmelt-mediated responses of DOC export to winter-time temperature fluctuations can impact surface water chemistry in forested watersheds by changing pH and aluminum transport.

6999

### **N<sub>2</sub>O Emissions from Streams in the Neuse River Watershed, North Carolina**

Craig A. Stow, John T. Walker, Lynette Cardoch, Porche Spence, and Chris Geron

Nitrous oxide emissions from the Neuse River and tributaries show a relationship with nitrate concentration that is consistent with previously reported results from other river systems.

■ 7005

### **Toxaphene Deposition to Lake Ontario via Precipitation, 1994–1998**

Deborah A. Burniston, William M. J. Strachan, and Robert J. Wilkinson

Precipitation samples taken from the master station site at Point Petre for the years 1996–1998 were analyzed for toxaphene and were used to determine wet loading of this analyte into Lake Ontario.

7012

### **Molecular Tracers of Saturated and Polycyclic Aromatic Hydrocarbon Inputs into Central Park Lake, New York City**

Beizhan Yan, Teofilo A. Abrajano, Richard F. Bopp, Damon A. Chaky, Lucille A. Benedict, and Steven N. Chillrud

Saturated and PAH markers in a sediment core from Central Park Lake reveal centennial and decadal shifts in energy use in New York City.

7020

### **Concentrations and Fluxes of Salmon-Derived Polychlorinated Biphenyls (PCBs) in Lake Sediments**

Eva M. Krümmel, Irene Gregory-Eaves, Robie W. Macdonald, Lynda E. Kimpe, Marc J. Demers, John P. Smol, Bruce Finney, and Jules M. Blais

A detailed survey of lake sediments shows that anadromous salmon are important vectors that transport PCBs from oceans to freshwater lakes in Alaska and British Columbia.

7027

### **Polybrominated Diphenyl Ethers in Indoor Dust in Ottawa, Canada: Implications for Sources and Exposure**

Bryony H. Wilford, Mahiba Shoeib, Tom Harner, Jiping Zhu, and Kevin C. Jones

Household dust may represent a significant addition to human PBDE exposure, particularly for children, and therefore should be considered for regulatory purposes. Dusts also constitute a diffuse regional source.

7036

### **Secondary Organic Aerosol Production from Terpene Ozonolysis. 1. Effect of UV Radiation**

Albert A. Presto, Kara E. Huff Hartz, and Neil M. Donahue

Aerosol production from the reaction of  $\alpha$ -pinene with ozone is shown to decrease in the presence of UV light; these results suggest that atmospheric aerosol production may depend significantly upon actinic flux.

7046

### **Secondary Organic Aerosol Production from Terpene Ozonolysis. 2. Effect of NO<sub>x</sub> Concentration**

Albert A. Presto, Kara E. Huff Hartz, and Neil M. Donahue

Compared with NO<sub>x</sub>-free conditions, adding NO<sub>x</sub> to the  $\alpha$ -pinene-ozone reaction system results in more volatile product distribution and therefore in reduced aerosol yields.

■ 7055

### **Distribution of Colloid Particles onto Interfaces in Partially Saturated Sand**

Yuniati Zevi, Annette Dathe, John F. McCarthy, Brian K. Richards, and Tammo S. Steenhuis

Direct visualization studies with bright-field and confocal laser microscopy give insights into the retention of colloids on phase interfaces in partially saturated sand.

■ 7065

### **Interactions of Fluoroquinolone Antibacterial Agents with Aqueous Chlorine: Reaction Kinetics, Mechanisms, and Transformation Pathways**

Michael C. Dodd, Amisha D. Shah, Urs von Gunten, and Ching-Hua Huang

Kinetic and mechanistic studies are used to evaluate fluoroquinolone interactions with aqueous chlorine; the results illustrate important differences between reactions mediated by secondary and tertiary amines.

■ 7077

### **Uranium Reduction in Sediments under Diffusion-Limited Transport of Organic Carbon**

Tetsu K. Tokunaga, Jiamin Wan, Jasquelin Pena, Eoin L. Brodie, Mary K. Firestone, Terry C. Hazen, Steve R. Sutton, Antonio Lanzarotti, and Matthew Newville

Uranium oxidation states (IV and VI) and microbial communities become stratified over short (cm) distances in sediments where organic carbon is diffusion-limited.

7084

### **Effect of pH and Aging Time on the Kinetic Dissociation of <sup>243</sup>Am(III) from Humic Acid-Coated $\gamma$ -Al<sub>2</sub>O<sub>3</sub>: A Chelating Resin Exchange Study**

Xiangke Wang, Changlun Chen, Jinzhou Du, Xiaoli Tan, Di Xu, and Shaoming Yu

Factors influencing the dissociation of Am<sup>3+</sup> from a humic acid-coated mineral surface are investigated.

■ 7089

### **Exposure–Effect Model for Calculating Copper Effect Concentrations in Sediments with Varying Copper Binding Properties: A Synthesis**

Stuart L. Simpson

An exposure–effect model and contaminant biodynamics show that “single-value” sediment quality guideline concen-

trations will be ineffective for predicting the toxicity of contaminants in sediment.

## 7097

### The Photolysis of Dihalomethanes in Surface Seawater

Manuela Martino, Peter S. Liss, and John M. C. Plane

Quantitative information is presented on photodegradation rates of  $\text{CH}_2\text{I}_2$ ,  $\text{CH}_2\text{BrI}$ , and  $\text{CH}_2\text{ClI}$  from systematic laboratory photochemical experiments carried out in artificial and natural seawater.

## 7102

### Adsorption, Oxidation, and Bioaccessibility of As(III) in Soils

Jae-Kyu Yang, Mark O. Barnett, Jinling Zhuang, Scott E. Fendorf, and Philip M. Jardine

The properties controlling the adsorption, oxidation, and bioaccessibility of As(III) in soils are examined, and a model to predict oral bioavailability is tested.

## 7111

### Effect of Alcohols on the Retention Mechanisms of Cd and Zn on Wyoming Bentonite and Illite

Rafiq K. Srour and Louis M. McDonald

Methanol- and ethanol-water mixtures decrease the partitioning of zinc onto bentonite and illite (after 10% alcohol) except in ethanol-water on illite, while cadmium remains unaffected.

## 7118

### Sources and Processes Affecting Sulfate in a Karstic Groundwater System of the Franconian Alb, Southern Germany

Florian Einsiedl and Bernhard Mayer

Sulfate in karst groundwater of the Franconian Alb is derived from atmospheric deposition and is affected by bacterial sulfate reduction at mean residence times of >60 years.

## 7126

### Impact of Ferrihydrite and Anthraquinone-2,6-Disulfonate on the Reductive Transformation of 2,4,6-Trinitrotoluene by a Gram-Positive Fermenting Bacterium

Thomas Borch, William P. Inskeep, Jace A. Harwood, and Robin Gerlach

A fermentive organism reduces TNT along different metabolite trajectories, depending on the presence of electron-shuttling compounds and surface-associated ferrous iron.

## 7134

### Biogeochemical Controls on Diel Cycling of Stable Isotopes of Dissolved $\text{O}_2$ and Dissolved Inorganic Carbon in the Big Hole River, Montana

Stephen R. Parker, Simon R. Poulson, Christopher H. Gammons, and Michael D. DeGrandpre

Diel changes in  $\delta^{18}\text{O}$ -DO and  $\delta^{13}\text{C}$ -DIC are demonstrated that were due to the effects of photosynthesis and respiration on dissolved oxygen and inorganic carbon.

## 7141

### Acid-Base Properties of Humic and Fulvic Acids Formed during Composting

César Plaza, Nicola Senesi, Alfredo Polo, and Gennaro Brunetti

During composting, organic materials form humic-like and fulvic-like acids, which possess an enhanced capacity to retain and exchange cations.

## 7147

### Competing Fe(II)-Induced Mineralization Pathways of Ferrihydrite

Colleen M. Hansel, Shawn G. Benner, and Scott Fendorf

Conversion of ferrihydrite to lepidocrocite, goethite, or magnetite is dictated by the kinetics of Fe(II) concentration, pH-, and ligand-dependent competing mineralization pathways.

## 7154

### Life Stage Specific Impact of Dimethoate on the Predatory Mite *Hypoaspis aculeifer* Canestrini (Gamasida: Laelapidae)

Lars-Henrik Heckmann, Kristine Maraldo, and Paul Henning Krogh

The "black box" of a soil mite reproductive test revealed that sensitivity decreases with the life stages: larvae > protonymphs > males > deutonymphs > females.

## 7158

### EDTA Degradation Induced by Oxygen Activation in a Zerovalent Iron/Air/Water System

Christina E. Noradoun and I. Francis Cheng

The room-temperature and atmospheric-pressure activation of oxygen is demonstrated; this process is used to degrade ethylenediaminetetraacetic acid.

## Environmental Modeling

### 7164

#### Errors in NAPL Volume Estimates Due to Systematic Measurement Errors during Partitioning Tracer Tests

Michael C. Brooks and William R. Wise

Uncertainty is determined due to random errors in volume and concentration measurements during moment-based analyses of partitioning tracer tests for nonaqueous-phase liquid volume estimation.

### 7170

#### Uncertainty in NAPL Volume Estimates Due to Random Measurement Errors during Partitioning Tracer Tests

Michael C. Brooks and William R. Wise

Errors are propagated for systematic errors in constant volume, proportional volume, and constant concentration during moment-based analyses of partitioning tracer tests for nonaqueous-phase liquid volume estimation.

## 7176

### Modeling of the Solid-Solution Partitioning of Heavy Metals and Arsenic in Embanked Flood Plain Soils of the Rivers Rhine and Meuse

Thomas J. Schröder, Tjisse Hiemstra, Jos P. M. Vink, and Sjoerd E. A. T. M. van der Zee

The possibility is assessed of predicting the solid-solution partitioning of heavy metals by a fully parameterized geochemical model.

## 7185

### Does the Forest Filter Effect Prevent Semivolatile Organic Compounds from Reaching the Arctic?

Yushan Su and Frank Wania

Global model calculations suggest that organic contaminant concentrations in the Arctic would be higher by as much as a factor of two without the filtering effect of forests.

## Environmental Measurements Methods

### 7194

#### Field-Scale Evaluation of the Passive Flux Meter for Simultaneous Measurement of Groundwater and Contaminant Fluxes

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