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# ENVIRONMENTAL Science & Technology

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*The Origin of Naturally Occurring  
Perchlorate: **The Role of  
ATMOSPHERIC Processes***

Field Trial of Transgenic Indian Mustard Plants

Allocating Cleanup Costs at Hazardous Waste Sites

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## Characterization of Natural and Affected Environments

1393

### On-Line Analysis of Gas-Phase Composition in the Combustion Chamber and Particle Emission Characteristics during Combustion of Wood and Waste in a Small Batch Reactor

T. Ferge, J. Maguhn, K. Hafner, F. Mühlberger, M. Davidovic, R. Warnecke, and R. Zimmermann

The impact of combustion conditions on the profile of gaseous pollutants in the combustion chamber as well as the particulate matter emission profile is investigated.

1403

### Temporal Changes in U.S. Benzene Emissions Inferred from Atmospheric Measurements

Tara J. Fortin, Benjamin J. Howard, David D. Parrish, Paul D. Goldan, William C. Kuster, Eliot L. Atlas, and Robert A. Harley

Various ambient measurements of benzene and acetylene are used to determine that benzene emissions decrease as a result of regulatory efforts.

1409

### Single-Particle Characterization of Four "Asian Dust" Samples Collected in Korea, Using Low-Z Particle Electron Probe X-ray Microanalysis

Chul-Un Ro, HeeJin Hwang, HyeKyeong Kim, Youngsin Chun, and René Van Grieken

Low-Z particle EPMA can provide more conclusive and detailed analysis of the chemical composition of Asian Dust particles than single-particle analysis with conventional EPMA.

1420

### Co-Occurrence of Triclocarban and Triclosan in U.S. Water Resources

Rolf U. Halden and Daniel H. Paull

An empirical model predicts nationwide contamination of U.S. water resources with 3,4,4'-trichlorocarbanilide, a toxic antimicrobial that has been mass-produced for decades.

1427

### Estrogenic Activity in Sediments from European Mountain Lakes

Natalia Garcia-Reyero, Benjamin Piña, Joan O. Grimalt, Pilar Fernández, Roger Fonts, Oliva Polvillo, and Belen Martrat

Recombinant yeast analyses show that sediment samples from high-altitude lakes exhibit significant estrogenic activity that is related to anthropogenic compounds deposited in these sites.

1436

### Emission Factors and Importance of PCDD/Fs, PCBs, PCNs, PAHs and PM<sub>10</sub> from the Domestic Burning of Coal and Wood in the U.K.

Robert G. M. Lee, Peter Coleman, Joanne L. Jones, Kevin C. Jones, and Rainer Lohmann

Emission factors for organic pollutants are determined from controlled coal and wood burning and compared to ambient profiles, and the potential contribution to national emissions is assessed.

1448

### Comparison of Toxaphene Congeners Levels in Five Seal Species from Eastern Canada: What Is the Importance of Biological Factors?

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Bruno Gouteux, Michel Lebeuf, Mike O. Hammill, Derek C. G. Muir, and Jean-Pierre Gagné

Diet is likely the main biological factor accounting for the large interspecies variations in toxaphene contamination of seals from eastern Canada.

1455

### Freshwater Mussel Shells as Environmental Chronicles: Geochemical and Taphonomic Signatures of Mercury-Related Extirpations in the North Fork Holston River, Virginia

Megan E. Brown, Michal Kowalewski, Richard J. Neves, Donald S. Cherry, and Madeline E. Schreiber

Geochemical and taphonomic signatures of freshwater mussel shells are used to assess spatial patterns of mercury contamination along the North Fork Holston River.

1463

### Spatial Variation of Streamwater Chemistry in Two Swedish Boreal Catchments: Implications for Environmental Assessment

Johan Temnerud and Kevin Bishop

This study highlights the importance of accounting for the spatial variability of water chemistry in headwater streams when assessing aquatic ecosystems in a landscape perspective.

1470

### PCBs and OCPs in Sediment Cores from the Lower St. Lawrence Estuary, Canada: Evidence of Fluvial Inputs and Time Lag in Delivery to Coring Sites

Michel Lebeuf and Teresa Nunes

Peak inputs of POPs apparently occurred after the period of maximum sales and production; this suggests a time lag in delivery of POPs to the sediments.

1479

### Molecular Characterization of Biodegradable Dissolved Organic Matter Using Bioreactors and [<sup>12</sup>C/<sup>13</sup>C] Tetramethylammonium Hydroxide Thermochemolysis GC-MS

Scott W. Frazier, Louis A. Kaplan, and Patrick G. Hatcher

TMAH thermochemolysis is used to observe changes in streamwater dissolved organic matter during passage through a bioreactor (namely, alteration of lignin and fatty acid components).

1492

### Use of Transplanted Zebra Mussels (*Dreissena polymorpha*) To Assess the Bioavailability of Microcontaminants in Flemish Surface Waters

Lieven Bervoets, Judith Voets, Adrian Covaci, Shaogang Chu, Diab Qadah, Roel Smolders, Paul Schepens, and Ronny Blust

Although BAFs/BSAFs do not predict bioaccumulation, measurements in transplanted zebra mussels should provide environmental managers with important additional information on the bioavailability of micropollutants.

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

■ 1506

### Colloid Stability in Vadose Zone Hanford Sediments

Szabolcs Czigány, Markus Flury, and James B. Harsh

Colloids in the vadose zone of the Hanford site form stable suspensions but have little chance to reach groundwater levels.

1513

### Growth Dilution of Metals in Microalgal Biofilms

Walter R. Hill and Ingvar L. Larsen

Laboratory and field experiments show the potential for variable algal growth rates to influence contaminant movement into aquatic food webs.

■ 1519

### Evidence for Anthropogenic $^{210}\text{Po}$ in the Urban Atmosphere of Seoul, Korea

Guebuem Kim, Young-Lim Hong, Jaeho Jang, Insung Lee, Dong-Woon Hwang, and Han-Soeb Yang

A correlation between non-sea-salt sulfate and excess  $^{210}\text{Po}$  suggests control by the same factor; the  $\delta S$  values indicate that the major source is probably anthropogenic.

1523

### Occurrence and Solid-Liquid Partition of Sulfonated Naphthalene-Formaldehyde Condensates in the Aquatic Environment

Frank T. Lange, Michael Merklinger, Michael Wenz, Heinz-J. Brauch, Markus Lehmann, and Istvan Pinter

Sulfonated naphthalene-formaldehyde condensates occur in wastewater and in German rivers and strongly adsorb to sewage sludge and riverine suspended solids and sediments.

## Environmental Processes

1532

### Heterogeneous Reactions of Glyoxal on Particulate Matter: Identification of Acetals and Sulfate Esters

John Liggio, Shao-Meng Li, and Robert McLaren

Evidence is presented that organic sulfates form in particles; results suggest that these products can contribute significantly to secondary organic aerosol.

1542

### Copper Toxicity to Larval Stages of Three Marine Invertebrates and Copper Complexation Capacity in San Diego Bay, California

Ignacio Rivera-Duarte, Gunther Rosen, David Lapota, David B. Chadwick, Lora Kear-Padilla, and Alberto Zirino

Copper complexation capacity keeps the free copper ion concentration below harmful levels for normal development of marine invertebrate larvae in San Diego Bay.

■ 1547

### Speciation of Mercury and Mode of Transport from Placer Gold Mine Tailings

Aaron J. Slowey, James J. Rytuba, and Gordon E. Brown, Jr.

Release of mercury from placer gold mine tailings used to hydrologically restore riverways poses a risk of mercury contamination to surrounding water bodies.

1555

### Hygroscopicity of Water-Soluble Organic Compounds in Atmospheric Aerosols: Amino Acids and Biomass Burning Derived Organic Species

Man Nin Chan, Man Yee Choi, Nga Lee Ng, and Chak K. Chan

The findings of this paper are useful for hygroscopic closure analysis when field measurements of aerosol composition and aerosol hygroscopic growth are available.

1563

### Vapor-Phase Exchange of Perchloroethene between Soil and Plants

Garrett C. Struckhoff, Joel G. Burken, and John G. Schumacher

Tree core sampling delineates an urban VOC plume prior to well placement, and associated laboratory studies lead to the discovery that vapor-phase uptake occurs.

1569

### The Origin of Naturally Occurring Perchlorate: The Role of Atmospheric Processes

Purnendu K. Dasgupta, P. Kalyani Martinelango, W. Andrew Jackson, Todd A. Anderson, Kang Tian, Richard W. Tock, and Srinath Rajagopalan

Traces of perchlorate can be found in rain or snow and can be produced from chloride by electrical discharge or ozone exposure.

1576

### Organic Complexation of Fe(II) and Its Impact on the Redox Cycling of Iron in Rain

R. J. Kieber, S. A. Skrabal, B. J. Smith, and J. D. Willey

Complexation by strong organic ligands plays an important role in the speciation of both Fe(II) and Fe(III) in rainwater.

1584

### Bioaerosol Emission Rate and Plume Characteristics during Land Application of Liquid Class B Biosolids

Benjamin D. Tanner, John P. Brooks, Charles N. Haas, Charles P. Gerba, and Ian L. Pepper

The rate of aerosolization of microorganisms during biosolids application is determined, and the effectiveness is investigated of microbially seeded groundwater as a novel model system.

1591

### Desorption Kinetics of Cd, Zn, and Ni Measured in Soils by DGT

H. Ernstberger, H. Zhang, A. Tye, S. Young, and W. Davison

Measurements using diffusive gradients in thin films show that release of nickel from solid phase to solution in soils is slower than the release of cadmium and zinc.

1598

### Remediation of Polycyclic Aromatic Hydrocarbon Compounds in Groundwater Using Poplar Trees

Mark A. Widdowson, Sandra Shearer, Rikke G. Andersen, and John T. Novak

The effectiveness of hybrid poplar trees in remediating PAH compounds is investigated.

1606

### Characterization of Charcoal Adsorption Sites for Aromatic Compounds: Insights Drawn from Single-Solute and Bi-Solute Competitive Experiments

Michael Sander and Joseph J. Pignatello

Although they share the same sites, nitrobenzene has greater intrinsic affinity for the surface than benzene and toluene; this is attributable to  $\pi$ - $\pi$  electron donor-acceptor interactions.

1616

### Biodegradability of Fractions of Dissolved Organic Carbon Leached from Decomposing Leaf Litter

Robert G. Qualls

Biodegradability of  $^{14}\text{C}$ -labeled natural dissolved organic matter is tested. Humic, fulvic, and hydrophilic acid fractions mineralize very slowly, and the hydrophilic neutral fraction mineralizes relatively rapidly.

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

**1623****Solubility of Hydrophobic Organic Pollutants in Binary and Multicomponent Aqueous Solvents**

E. Ruckenstein and I. Shulgin

The solubilities of hydrophobic pollutants in binary and multicomponent aqueous solvents are examined in the framework of the fluctuation theory of solution.

**1632****Atmospheric Chemistry of Hydrazoic Acid (HN<sub>3</sub>): UV Absorption Spectrum, HO• Reaction Rate, and Reactions of the •N<sub>3</sub> Radical**

John J. Orlando, Geoffrey S. Tyndall, Eric A. Betterton, Joe Lowry, and Steve T. Stegall

The diurnally averaged tropospheric lifetime of HN<sub>3</sub> is ~1–2 days, with both solar photolysis and reaction with HO• contributing about equally to its removal.

**1641****Influence of Addition Order and Contact Time on Thorium(IV) Retention by Hematite in the Presence of Humic Acids**

Pascal Reiller, Florence Casanova, and Valérie Moulin

The influence of the addition order in this system is experimentally evidenced and discussed for tetravalent elements that are relevant for the reduced state of actinides.

**1649****Sorption Kinetics of Organic Contaminants by Sandy Aquifer and Its Kerogen Isolate**

Yong Ran, Baoshan Xing, P. Suresh C. Rao, Guoying Sheng, and Jiamo Fu

The sorption equilibrium times (over one decade) for phenanthrene on the Borden aquifer and its kerogen isolate are much longer than previously understood.

**1658****Nonmonotonic Variations in Deposition Rate Coefficients of Microspheres in Porous Media under Unfavorable Deposition Conditions**

Xiqing Li and William P. Johnson

Colloid deposition rate coefficients are demonstrated to vary nonmonotonically with distance from source even under unfavorable deposition conditions with simple solution chemistries.

**1666****Effect of Algal and Bacterial Diet on Methyl Mercury Concentrations in Zooplankton**

Martin Kainz and Asit Mazumder

Methyl mercury concentrations in zooplankton are significantly predicted by retention of bacterial and, to a lesser degree, algal diet.

**1673****Protein Nitration by Polluted Air**

Thomas Franze, Michael G. Weller, Reinhard Niessner, and Ulrich Pöschl

Proteins are efficiently nitrated by polluted air under summer smog conditions; this provides a molecular rationale for the promotion of allergies by traffic-related air pollution.

**1679****Determination of Mercury Evasion in a Contaminated Headwater Stream**

Antu C. Maprani, Tom A. Al, Kerry T. MacQuarrie, John A. Dalziel, Sean A. Shaw, and Phillip A. Yeats

A method for integrated measurement of mercury evasion along streams is presented as an alternative to point-measurement techniques in which uncertainty results from in-stream variability.

**1688****Sorption of Ionic Surfactants to Estuarine Sediment and Their Influence on the Sequestration of Phenanthrene**

Tracey Jones-Hughes and Andrew Turner

Differences in the nature and extent of cationic and anionic surfactant sorption to estuarine sediment result in different effects on the sorption of phenanthrene.

**1698****Dissolution-Induced Contact Angle Modification in Dense Nonaqueous Phase Liquid/Water Systems**

Orphius I. Mohammad and Tohren C. G. Kibbey

Long-term dissolution experiments and drop shape modeling are used to study the effects of dissolution and drop pinning on the contact angles of DNAPL drops.

**Environmental Modeling****1707****Use of Personal–Indoor–Outdoor Sulfur Concentrations to Estimate the Infiltration Factor and Outdoor Exposure Factor for Individual Homes and Persons**

Lance Wallace and Ron Williams

The contribution of outdoor particles to personal exposure for a group of 37 persons monitored one week per season over four seasons in 2000–2001 is estimated.

**1715****Comparison between Back-Trajectory Based Modeling and Lagrangian Backward Dispersion Modeling for Locating Sources of Reactive Gaseous Mercury**

Young-Ji Han, Thomas M. Holsen, Philip K. Hopke, and Seung-Muk Yi

RGM sources include coal-fired power plants in New York and Pennsylvania, a large copper smelter in Quebec, and taconite mining areas around the Great Lakes.

**1724****Calculations of Incremental Secondary Organic Aerosol Reactivity**

Marc Carreras-Sospedra, Robert J. Griffin, and Donald Dabdup

Regression analysis is used to determine values for incremental secondary organic aerosol reactivity in the California South Coast Air Basin; values at individual locations are also reported.

**Environmental Measurements Methods****1731****Comparison of Centrifugation and Filtration Techniques for the Size Fractionation of Colloidal Material in Soil Suspensions Using Sedimentation Field-Flow Fractionation**

Laura J. Gimbert, Philip M. Haygarth, Ronald Beckett, and Paul J. Worsfold

Sedimentation field-flow fractionation is used to investigate and compare colloidal fractions of soil solutions isolated by centrifugation and membrane filtration techniques.

**1736****Structure of the Toxaphene Compound 2,5-endo,6-exo,8,9,9,10,10-Octachlorobornene-2: A Temperature-Dependent Formation of Two Rotamers**

Harun Parlar, Jürgen Burhenne, Mehmet Coelhan, and Walter Vetter

For the first time, spectroscopic analyses of the toxaphene compound 2,5-endo,6-exo,8,9,9,10,10-octachlorobornene-2 show that two rotamers form at low temperatures.