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# ENVIRONMENTAL Science & Technology

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## Electrochemically Assisted **MICROBIAL** Production of Hydrogen

Perchlorate Biodegradation for Water Treatment

Quantitative Determination of Perfluorochemicals  
in Sediments and Sludge

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THE AMERICAN  
CHEMICAL SOCIETY

## Characterization of Natural and Affected Environments

■ 3889

### Halogenated Natural Products in Five Species of Antarctic Sponges: Compounds with POP-like Properties?

Walter Vetter and Dorte Janussen

More than 100 halogenated natural products suspected to show POP-like properties are found in 5 species of Antarctic sponges.

3896

### ELISA as an Affordable Methodology for Monitoring Groundwater Contamination by Pesticides in Low-Income Countries

Beatriz M. Brena, Lourdes Arellano, Caterina Rufo, Michael S. Last, Jorge Montaña, Eduardo Egaña Cerni, Gualberto Gonzalez-Sapienza, and Jerold A. Last

Over a 2-year period, ELISA was used to analyze groundwater simazine, atrazine, carbaryl, and 1-naphthol in an agricultural region of Uruguay; low levels of contamination are found.

■ 3904

### Exposure Assessment and Risk Characterization for Perfluorooctanoate in Selected Consumer Articles

Stephen T. Washburn, Timothy S. Bingman, Scott K. Braithwaite, Robert C. Buck, L. William Buxton, Harvey J. Clewell, Lynne A. Haroun, Janet E. Kester, Robert W. Rickard, and Annette M. Shipp

The potential human health significance of trace levels of perfluorooctanoate ( $C_8F_{15}O_2$ ) detected in certain consumer articles is assessed.

3911

### Source Apportionment of Organic Pollutants of a Highway-Traffic-Influenced Urban Area in Bayreuth (Germany) Using Biomarker and Stable Carbon Isotope Signatures

Bruno Glaser, Annekatrin Dreyer, Michael Bock, Stefan Fiedler, Marion Mehring, and Tobias Heitmann

Biomarker and stable carbon isotope signatures are used to differentiate traffic- and urban-derived black carbon and PAH contamination.

3918

### Long-Term Change of Polycyclic Aromatic Hydrocarbon Deposition to Peatlands of Eastern Canada

Annekatrin Dreyer, Michael Radke, Jukka Turunen, and Christian Blodau

Historic deposition rates of PAH to 17 ombrotrophic peatlands of eastern Canada are determined for the period of about 1850–2000.

3925

### Investigation of the Role of Structural Domains Identified in Sedimentary Organic Matter in the Sorption of Hydrophobic Organic Compounds

Christopher J. Golding, Ronald J. Smernik, and Gavin F. Birch

Novel  $^{13}C$  NMR techniques determine that distinct structural domains in estuarine sedimentary organic matter do not have the same affinity for a common hydrophobic compound.

■ 3933

### Investigations of the Potential Influence of Environmental Contaminants on the Thymus and Spleen of Harbor Porpoises (*Phocoena phocoena*)

Andreas Beineke, Ursula Siebert, Michael McLachlan, Regina Bruhn, Kristina Thron, Klaus Failing, Gundi Müller, and Wolfgang Baumgärtner

The influence of environmental contaminants on lymphoid organs of the harbor porpoise is presented.

3939

### Gas Transport below Artificial Recharge Ponds: Insights from Dissolved Noble Gases and a Dual Gas ( $SF_6$ and $^3He$ ) Tracer Experiment

Jordan F. Clark, G. Bryant Hudson, and Dror Avisar

Trapped air did not significantly affect the transport of gas tracers through the unsaturated zone beneath an artificial recharge pond with a high infiltration rate.

■ 3946

### Quantitative Determination of Perfluorochemicals in Sediments and Domestic Sludge

Christopher P. Higgins, Jennifer A. Field, Craig S. Criddle, and Richard G. Luthy

Analysis of sediments and sewage sludges shows widespread distribution of anionic perfluorochemicals at low concentrations.

3957

### Determination of Temperature-Dependent Henry's Law Constants of Odorous Contaminants and Their Application to Human Perception

Pinar Ömür-Özbek and Andrea M. Dietrich

Odorous aqueous pollutants are problematic to consumers, and a new method is presented for determining the contaminants' Henry's law constants and enthalpies of aqueous vaporization.

3964

### Selected Volatile Organic Compounds in Residential Air in the City of Ottawa, Canada

Jiping Zhu, Ron Newhook, Leonora Marro, and Cecilia C. Chan

Active sampling and thermal desorption GC/MS analysis are used to measure volatile organic compounds in indoor and outdoor air in randomly selected residences in Ottawa, Canada.

## Environmental Processes

3972

### Comparative Effects of Dietary Methylmercury on Gene Expression in Liver, Skeletal Muscle, and Brain of the Zebrafish (*Danio rerio*)

P. Gonzalez, Y. Dominique, J. C. Massabuau, A. Boudou, and J. P. Bourdineaud

Effects are presented of dietary methylmercury on gene expression in the liver, skeletal muscle, and brain of the zebrafish contaminated at 5- and 13.5- $\mu g$  of Hg/g.

3981

### Occurrence and Sorption Behavior of Sulfonamides, Macrolides, and Trimethoprim in Activated Sludge Treatment

Anke Göbel, Angela Thomsen, Christa S. McArdell, Adriano Joss, and Walter Giger

Intensive mass balance studies show that the sorption to sludge of sulfonamides, macrolides, and trimethoprim is of minor importance.

3990

### Adsorption of Single-Ring Organic Compounds to Wood Charcoals Prepared under Different Thermochemical Conditions

Dongqiang Zhu, Seokjoon Kwon, and Joseph J. Pignatello

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

Adsorption intensity is greater for polar than apolar solutes but decreases with surface oxygen functionality for all solutes because of competition for adsorption space by water molecules.

**3999**

### Temperature and Congener Structure Affect the Enantioselectivity of Toxaphene Elimination by Fish

Keith A. Maruya, Kelly L. Smalling, and Walter Vetter

A new classification is presented for toxaphene congeners based on temperature-dependent, enantioselective elimination by a model estuarine fish.

**4005**

### Enhanced Biodegradation of $\beta$ - and $\delta$ -Hexachlorocyclohexane in the Presence of $\alpha$ - and $\gamma$ -Isomers in Contaminated Soils

Manish Kumar, Pankaj Chaudhary, Manish Dwivedi, Ranjan Kumar, Debarati Paul, Rakesh K. Jain, Satyendra K. Garg, and Ashwani Kumar

The isolate *Pseudomonas aeruginosa* ITRC-5 can be used for the remediation of sites contaminated with different isomers of the chlorinated insecticide hexachlorocyclohexane.

**4012**

### Role of Hydrodynamic Drag on Microsphere Deposition and Re-Entrainment in Porous Media under Unfavorable Conditions

Xiqing Li, Pengfei Zhang, C. L. Lin, and William P. Johnson

The role of hydrodynamic drag in mitigating colloid deposition and enhancing colloid re-entrainment in porous media under unfavorable deposition conditions is examined.

**4021**

### Understanding the Difference in Oxidative Properties between Flame and Diesel Soot Nanoparticles: The Role of Metals

S. H. Kim, R. A. Fletcher, and M. R. Zachariah

The differences in the oxidative kinetics between flame- and diesel-derived soot are observed.

■ **4027**

### Effect of Soil Fulvic Acid on Nickel(II) Sorption and Bonding at the Aqueous-Boehmite ( $\gamma$ -AlOOH) Interface

Timothy J. Strathmann and Satish C. B. Myneni

Both the extent of Ni(II) sorption by boehmite and the local structures of the sorbing Ni(II) surface complexes are modified by co-sorption of fulvic acid.

**4035**

### Similarities between Inorganic Sulfide and the Strong Hg(II)-Complexing Ligands in Municipal Wastewater Effluent

Heileen Hsu-Kim and David L. Sedlak

Speciation and oxidation experiments with model sulfide ligands indicate that dissolved Hg speciation in wastewater effluent is dominated by inorganic sulfide.

■ **4042**

### Sorption Mechanisms of Zinc on Hydroxyapatite: Systematic Uptake Studies and EXAFS Spectroscopy Analysis

Young J. Lee, Evert J. Elzinga, and Richard J. Reeder

Uptake experiments and EXAFS spectroscopy provide insight into mechanisms of Zn interaction with hydroxyapatite, revealing conditions that favor formation of surface adsorption complexes and Zn precipitates.

**4049**

### Contributions of Organic Peroxides to Secondary Aerosol Formed from Reactions of Monoterpenes with O<sub>3</sub>

Kenneth S. Docherty, Wilbur Wu, Yong Bin Lim, and Paul J. Ziemann

Laboratory studies indicate that organic peroxides comprise a major fraction of the secondary organic aerosol mass formed from reactions of monoterpenes with O<sub>3</sub>.

**4060**

### Surface Complexation Modeling of Proton and Cd Adsorption onto an Algal Cell Wall

Emily S. Kaulbach, Jennifer E. S. Szymanowski, and Jeremy B. Fein

A surface complexation modeling approach is used to quantify proton and Cd adsorption onto the cell wall of the algal species *Pseudokirchneriella subcapitata*.

**4066**

### Chemical Nitrite Oxidation in Acid Solutions as a Consequence of Microbial Ammonium Oxidation

Kai M. Udert, Tove A. Larsen, and Willi Gujer

Acid-tolerant ammonium-oxidizing bacteria trigger chemical nitrite oxidation in highly concentrated ammonium nitrite solutions.

**4076**

### Factors Affecting Acid Neutralizing Capacity in the Adirondack Region of New York: A Solute Mass Balance Approach

Mari Ito, Myron J. Mitchell, Charles T. Driscoll, and Karen M. Roy

Annual input-output budgets for major solutes and ANC are estimated for 43 watersheds, with the goal of evaluating the factors that affect the sensitivity of surface waters to acidic deposition.

■ **4082**

### Enhanced Dechlorination of Chlorinated Methanes and Ethenes by Chloride Green Rust in the Presence of Copper(II)

R. A. Maithreepala and Ruy-an Doong

The addition of Cu(II) to chloride green rust can effectively dechlorinate carbon tetrachloride, chloroform, tetrachloroethene, and trichloroethene under various environmental conditions.

**4091**

### Formation and Reaction of Hydroxycarbonyls from the Reaction of OH Radicals with 1,3-Butadiene and Isoprene

Jillian Baker, Janet Arey, and Roger Atkinson

Reaction products are investigated of hydroxyl radical-initiated reactions of atmospheric emissions of 1,3-butadiene and isoprene released from vehicle exhaust or vegetation.

**4100**

### Differential Potentiometric Titration: Development of a Methodology for Determining the Point of Zero Charge of Metal (Hydr)oxides by One Titration Curve

Kyriakos Bourikas, Christos Kordulis, and Alexis Lycourghiotis

Differential potentiometric titration allows the determination of the point of zero charge of metal hydroxides from the inflection point of only one potentiometric curve.

■ **4109**

### Effects of Progressive Anoxia on the Solubility of Technetium in Sediments

Ian T. Burke, Christopher Boothman, Jonathon R. Lloyd, Robert J. G. Mortimer, Francis R. Livens, and Katherine Morris

The development of anoxic conditions in estuarine sediment microcosms and their effects on pertechnetate solubility, microbial population, and the fate of technetium in these estuarine sediments are described.

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

4117

### Neptunium(V) Partitioning to Uranium(VI) Oxide and Peroxide Solids

Matthew Douglas, Sue B. Clark, Judah I. Friese, Bruce W. Arey, Edgar C. Buck, and Brady D. Hanson

Trace quantities of neptunium partition into metastudtite ( $\text{UO}_4 \cdot 4\text{H}_2\text{O}$ ) but not metaschoepite ( $[(\text{UO}_2)_8\text{O}_2(\text{OH})_{12}] \cdot 10\text{H}_2\text{O}$ ), although Np release from metastudtite exceeds congruent dissolution of the solid.

■ 4125

### Influence of Sediment Bioreduction and Reoxidation on Uranium Sorption

Chongxuan Liu, John M. Zachara, Lirong Zhong, Ravi Kukkadupa, Jim E. Szecsody, and Dave W. Kennedy

The complexity of the coupled U-Fe redox system is highlighted, and sorbed Fe(II) is not a universal reductant for U(VI), as commonly assumed.

4134

### Lake Restoration by Dosing Aluminum Relative to Mobile Phosphorus in the Sediment

Kasper Reitzel, Jonas Hansen, Frede O. Andersen, Kjeld S. Hansen, and Henning S. Jensen

The reduction of internal phosphorus loading by dosing aluminum relative to the mobile phosphorus pool in the sediment is investigated.

## Environmental Modeling

4141

### Modeling Photoinduced Algal Toxicity of Polycyclic Aromatic Hydrocarbons

Matthias Grote, Gerrit Schüürmann, and Rolf Altenburger

Photoinduced algal toxicity of PAHs can be described as a function of internal concentrations, absorbed amount of photons, and a compound-specific relative phototoxic efficacy value.

4150

### Evidence for the Stepwise Stress Model: *Gambusia holbrooki* and *Daphnia magna* under Acid Mine Drainage and Acidified Reference Water Stress

Almut Gerhardt, Luc Janssens de Bisthoven, and Amadeu M. V. Soares

The Stepwise Stress Model describes behavioral plasticity of aquatic species and can be used in biological early warning systems.

■ 4159

### Representation of Secondary Organic Aerosol Laboratory Chamber Data for the Interpretation of Mechanisms of Particle Growth

Jesse H. Kroll and John H. Seinfeld

Simplified models of gas-particle partitioning are used to describe laboratory growth data and apply them to atmospheric models.

■ 4166

### Effect of Lot Variability on Ultraviolet Radiation Inactivation Kinetics of *Cryptosporidium parvum* Oocysts

Mano Sivaganesan and Siva Sivaganesan

The estimated UV dose required to inactivate *Cryptosporidium parvum* is larger when lot variability is included in the regression model.

■ 4172

### Spatial Variability of Fine Particle Mass, Components, and Source Contributions during the Regional Air Pollution Study in St. Louis

Eugene Kim, Philip K. Hopke, Joseph P. Pinto, and William E. Wilson

A model that includes variables such as wind speed, wind direction, and season is used to identify sources and estimate the contribution of each source.

4180

### Model Demonstrating the Potential for Coupled Nitrification Denitrification in Soil Aggregates

Arie Kremen, Jacob Bear, Uri Shavit, and Avi Shavit

Diffusive constraints are controlling the existence and extent of anaerobic conditions in soil aggregates and thus are affecting the evolution of gaseous nitrogen.

■ 4189

### Quantification of Sequential Chlorinated Ethene Degradation by Use of a Reactive Transport Model Incorporating Isotope Fractionation

Boris M. Van Breukelen, Daniel Hunkeler, and Frank Volkering

Isotope fractionation reactive transport modeling improves quantification of sequential chlorinated ethene degradation as illustrated by microcosm, scenario, and field modeling.

## Environmental Measurements Methods

4198

### Quantification of Toxic *Microcystis* spp. during the 2003 and 2004 Blooms in Western Lake Erie using Quantitative Real-Time PCR

J. M. Rinta-Kanto, A. J. A. Ouellette, G. L. Boyer, M. R. Twiss, T. B. Bridgeman, and S. W. Wilhelm

Toxic cyanobacterium of *Microcystis* reoccurred at high abundance in Lake Erie since 1995, and molecular biology now provides an approach to quantitatively characterize these events.

4206

### Congener-Specific Carbon Isotopic Analysis of Technical PCB and PCN Mixtures Using Two-Dimensional Gas Chromatography-Isotope Ratio Mass Spectrometry

Yuichi Horii, Kurunthachalam Kannan, Gert Patrick, Toshitaka Gamo, Jerzy Falandysz, and Nobuyoshi Yamashita

Two-dimensional gas chromatography-isotope ratio mass spectrometry is used to conduct congener-specific carbon isotopic analyses of technical PCB and PCN mixtures.

4213

### High Time Resolution and Size-Segregated Analysis of Aerosol-Bound Polycyclic Aromatic Hydrocarbons

Christian Emmenegger, Markus Kalberer, Vera Samburova, and Renato Zenobi

High time resolution measurements are used to gain knowledge of the fate and diurnal patterns of PAHs in the atmosphere.

4220

### Sediment Dilution Method to Determine Sorption Coefficients of Hydrophobic Organic Chemicals

Thomas L. ter Laak, Philipp Mayer, Frans J. M. Busser, Hans J. C. Klamer, and Joop L. M. Hermens

This study presents a simple sediment dilution method to determine sorption coefficients of hydrophobic compounds to a spiked and field-contaminated sediment.

■ 4226

### Shifts in Relative Tissue $\delta^{15}\text{N}$ Values in Snowy Egret Nestlings with Dietary Mercury Exposure: A Marker for Increased Protein Degradation

Patricia L. Shaw-Allen, Christopher S. Romanek, A. L. Bryan, Jr., Heather Brant, and Charles H. Jago

Toxicant-mediated changes in tissue nitrogen isotope profiles are a sensitive indicator of stress; as a trophic resource, these shifts may help address hierarchical issues in ecotoxicology.

4234

**Analyte Peptidomimetics Selected from Phage Display Peptide Libraries: A Systematic Strategy for the Development of Environmental Immunoassays**

Soledad Cardozo, Andrés González-Techera, Jerold A. Last, Bruce D. Hammock, Karl Kramer, and Gualberto G. González-Sapienza

Analyte peptidomimetics selected from phage display peptide libraries can be used as advantageous substitutes for tracer reagents in the development of environmental immunoassays.

## Remediation and Control Technologies

4242

**Photocatalytic Reduction and Recovery of Mercury by Polyoxometalates**

E. Gkika, A. Troupis, A. Hiskia, and E. Papaconstantinou

Mercury concentrations from 20 to 800 ppm can be handled; this enables almost complete recovery of mercury, and the catalyst is not poisoned by metal precipitation.

4249

**Structure Characterization and Adsorption Properties of Pyrolyzed Sewage Sludge**

S. Rio, C. Faur-Brasquet, L. Le Coq, and P. Le Cloirec

Production of porous carbonaceous materials from sewage sludge by pyrolysis is investigated, with a goal of different industrial applications.

4258

**Fluctuations of Dissolved Organic Matter in River Used for Drinking Water and Impacts on Conventional Treatment Plant Performance**

Christian Volk, Louis A. Kaplan, Jeff Robinson, Bruce Johnson, Larry Wood, Hai Wei Zhu, and Mark LeChevallier

This study describes parameters that affect levels of organic matter in source water and removal during drinking-water treatment.

4265

**Combustion Properties and Desulfurization of High Sulfur Containing Indian and Nepali Coals Using Lime-Based Products**

Ramesh M. Singh, Mitsushi Kamide, Tianji Li, and Heejoon Kim

The physical and combustion characteristics of some Indian and Nepali coals are studied.

4270

**Microbial Passage in Low Pressure Membrane Elements with Compromised Integrity**

Baoxia Mi, Benito J. Mariñas, Jason Curl, Sandeep Sethi, Gil Crozes, and Dan Hugaboom

The passage of *Bacillus subtilis* spores through UF/MF membrane elements of compromised integrity installed in full-scale racks is investigated experimentally and simulated with a model.

4280

**Physicochemical Properties Related to Long-Term Phosphorus Retention by Drinking-Water Treatment Residuals**

Konstantinos C. Makris, Willie G. Harris, George A. O'Connor, Thomas A. Obreza, and Herschel A. Elliott

Long-term phosphorus sorption capacities for WTRs with different physicochemical properties are predicted on the basis of their specific surface area, porosity, and total C content.

4290

**Oxidation of Pharmaceuticals during Ozonation of Municipal Wastewater Effluents: A Pilot Study**

Marc M. Huber, Anke Göbel, Adriano Joss, Nadine Hermann, Dirk Löffler, Christa S. Mc Ardell, Achim Ried, Hansruedi Siegrist, Thomas A. Ternes, and Urs von Gunten

Pilot-scale ozonation of wastewater effluents shows that many pharmaceuticals are efficiently oxidized and that suspended solids have only minor effects on the oxidation of pharmaceuticals.

■ 4300

**Ineffectiveness and Poor Reliability of Arsenic Removal Plants in West Bengal, India**

M. Amir Hossain, Mrinal Kumar Sengupta, Sad Ahamed, Mohammad Mahmudur Rahman, Debapriya Mondal, Dilip Lodh, Bhaskar Das, Bishwajit Nayak, Bimal K. Roy, Amitava Mukherjee, and Dipankar Chakraborti

The efficiency of arsenic removal plants in an arsenic-affected area of West Bengal, India, is critically evaluated on the basis of a 2-year study.

## Sustainability Engineering and Green Chemistry

4307

▶ **C<sub>60</sub> in Water: Nanocrystal Formation and Microbial Response**

J. D. Fortner, D. Y. Lyon, C. M. Sayes, A. M. Boyd, J. C. Falkner, E. M. Hotze, L. B. Alemany, Y. J. Tao, W. Guo, K. D. Ausman, V. L. Colvin, and J. B. Hughes

These studies examine C<sub>60</sub> in water as stable nanoscale aggregates, with a focus on composition, formation dynamics, stability, and potential microbial inhibition.

4317

▶ **Electrochemically Assisted Microbial Production of Hydrogen from Acetate**

Hong Liu, Stephen Grot, and Bruce E. Logan

The augmentation of the potential of a completely anaerobic microbial fuel cell shows that microbial hydrogen production is possible from acetate.

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

▶ This issue contains a news story about this research.