December 15, 2006

# Environmental Science & Technology

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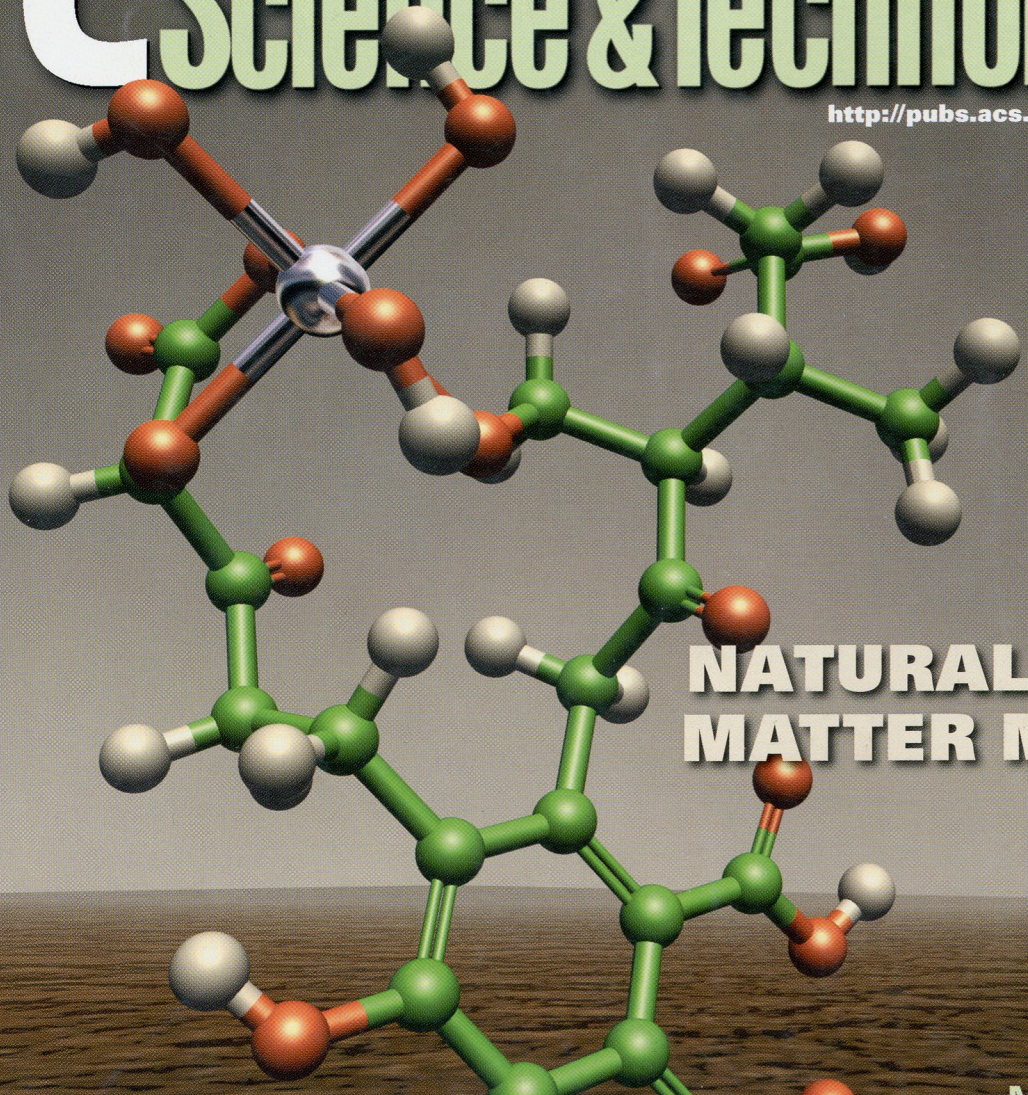


## NATURAL ORGANIC MATTER MODELING

PCBs and PBDEs in Indoor Air

New Nitrosamines in Drinking Water

PUBLISHED BY
THE AMERICAN
CHEMICAL SOCIETY

ENVIRONMENTAL Science & Technology

40(24) 7451–7988 : ISSN 0013 936X

December 15, 2006 • Vol. 40 No. 24



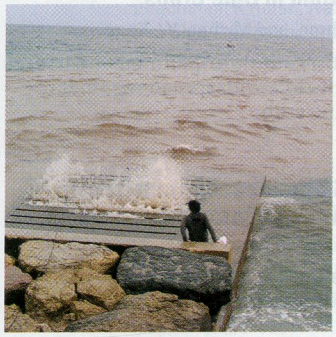
# News and Features

## NEWS



## FEATURE





The use of models to understand the speciation and distribution of metals in the environment is essential for predicting metal transport and bioavailability. The authors discuss primary metal–particle interaction models and point out their limitations. They also examine how predictions from models compare with field measurements.

# Research

## SPECIAL SECTION: NATURAL ORGANIC MATTER MODELING

Natural organic matter (NOM) plays a key role in rivers, lakes, groundwater, seawater, and soils for the binding of cations and for interactions with mineral surfaces. The complexity of the heterogeneous properties of NOM is a challenge to model development. The four manuscripts in this special section present some recent model developments that will improve our understanding of these complex interactions and provide a framework for application to natural systems. *ES&T* Associate Editor Laura Sigg served as the coordinator for this section.



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

**Cover:** Ken Eward of BioGrafx designed the cover image, which shows $Pb^{2+}$ interacting with natural organic matter.

**Online news:** Read news first at http://pubs.acs.org/estnews.

## CRITICAL REVIEWS



## CHARACTERIZATION OF NATURAL AND AFFECTED ENVIRONMENTS

The speciation of Cr within a soil by an approach based on physical soil fractionation before EXAFS speciation analyses is reported.

■ **7609**

**Characterizing the Redox Status in Three Different Forested Wetlands with Geochemical Data**

Christine Alewell, Sonja Paul, Gunnar Lischeid, Kirsten Küsel, and Matthias Gehre

Redox processes in forested wetlands (in Germany) demonstrate a high temporal and spatial heterogeneity; this indicates that the sequential reduction chain is not a suitable modeling concept.

**7616**

**Tracking Anthropogenic Inputs Using Caffeine, Indicator Bacteria, and Nutrients in Rural Freshwater and Urban Marine Systems**

Kelly A. Peeler, Stephen P. Opsahl, and Jeffrey P. Chanton

Caffeine, nutrients, and indicator bacteria were used to distinguish human versus nonhuman sources of surface-water contamination in rural freshwater and urban marine environments.

**7623**

**Hurricane Katrina's Impact on New Orleans Soils Treated with Low Lead Mississippi River Alluvium**

Howard W. Mielke, Eric T. Powell, Christopher R. Gonzales, and Paul W. Mielke, Jr.

Even after New Orleans was flooded, Mississippi River alluvial soil spread on contaminated properties remains stable and continues to provide lead-safe outdoor environments for children.

■ **7629**

**Factors Influencing the National Distribution of Polycyclic Aromatic Hydrocarbons and Polychlorinated Biphenyls in British Soils**

Elizabeth Heywood, Julian Wright, Claire L. Wienburg, Helaina I. J. Black, Sara M. Long, Dan Osborn, and David J. Spurgeon

Measurement of POP concentrations in soils illustrates the importance of source intensity for PAHs and of source intensity, long-range processes, and soil organic content for PCBs.

■ **7636**

▶ **Characterization of New Nitrosamines in Drinking Water Using Liquid Chromatography Tandem Mass Spectrometry**

Yuan-Yuan Zhao, Jessica Boyd, Steve E. Hrudey, and Xing-Fang Li

Two new disinfection byproducts NDPhA and NPip, along with NDMA and NPyr, are identified in a drinking-water distribution system by liquid chromatography/tandem mass spectrometry.

■ **7642**

**Perfluorooctanesulfonate and Related Fluorochemicals in Albatrosses, Elephant Seals, Penguins, and Polar Skuas from the Southern Ocean**

Lin Tao, Kurunthachalam Kannan, Natsuko Kajiwara, Mônica M. Costa, Gilberto Fillmann, Shin Takahashi, and Shinsuke Tanabe

Southern Ocean albatrosses and elephant seals contain 10–100-fold lower levels of perfluorochemicals than Arctic birds and seals.

**7649**

**Enantioselective Formation of Methyl Sulfone Metabolites of 2,2′,3,3′,4,6′-Hexachlorobiphenyl in Rat**

Karin Norström, Johan Eriksson, Johanna Haglund, Virginia Silvari, and Åke Bergman

Methyl sulfone metabolites of CB-132 are formed through an enantioselective process in the rat.

■ **7656**

**Tropospheric Phosphine and Its Sources in Coastal Antarctica**

Renbin Zhu, Deming Kong, Liguang Sun, Jinju Geng, Xiaorong Wang, and Dietmar Glindemann

The exploration of unexpectedly high atmospheric phosphine concentrations in coastal Antarctica is reported and is linked to soils of sea-animal colonies as emission sources.

## ENVIRONMENTAL PROCESSES

■ **7662**

**Kinetics of Contaminant Desorption from Soil: Comparison of Model Formulations Using the Akaike Information Criterion**

Christopher M. Saffron, Jeong-Hun Park, Bruce E. Dale, and Thomas C. Voice

The Akaike information criterion is used to select among nine mathematical models for the description of desorption rates for atrazine- and naphthalene-contaminated soils.

**7668**

**Oxidation of Aromatic and Aliphatic Hydrocarbons by OH Radicals Photochemically Generated from $H_2O_2$ in Ice**

Jindřiška Dolinová, Radovan Růžička, Romana Kurková, Jana Klánová, and Petr Klán

The study of oxidation of aromatic and saturated aliphatic hydrocarbons by the hydroxyl radicals, photochemically produced from hydrogen peroxide in ice, is described.

■ **7675**

**Effects of Trace Element Concentration on Enzyme Controlled Stable Isotope Fractionation during Aerobic Biodegradation of Toluene**

Silvia A. Mancini, Sarah K. Hirschorn, Martin Elsner, Georges Lacrampe-Couloume, Brent E. Sleep, Elizabeth A. Edwards, and Barbara Sherwood Lollar

Smaller isotopic fractionation during toluene biodegradation is observed for *Pseudomonas putida* mt-2 grown under high versus low iron concentrations; this is probably due to a change in enzyme kinetics.

**7682**

**Heterogeneous Reactions of Methylglyoxal in Acidic Media: Implications for Secondary Organic Aerosol Formation**

Jun Zhao, Nicholas P. Levitt, Renyi Zhang, and Jianmin Chen

Hydration and polymerization of methylglyoxal contribute to secondary organic aerosol formation; these are dependent on hygroscopicity, rather than acidity of the aerosols.

■ **7688**

**Influence of Surface Potential on Aggregation and Transport of Titania Nanoparticles**

Katherine A. Dunphy Guzman, Michael P. Finnegan, and Jillian F. Banfield

Aggregation and transport of titania nanoparticles under varying pH conditions are studied with micromodels, and the ability of theory to predict nanoparticle interactions is evaluated.

■ **7694**

**Sorption of Trichloroethylene in Hydrophobic Micropores of Dealuminated Y Zeolites and Natural Minerals**

Hefa Cheng and Martin Reinhard

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

Thermodynamic considerations and laboratory experiments suggest that trichloroethylene adsorbs into hydrophobic micropores of minerals by displacing loosely bound water; this process is driven primarily by enthalpic contributions.

■ **7702**

**Microscale Investigations of Ni Uptake by Cement Using a Combination of Scanning Electron Microscopy and Synchrotron-Based Techniques**

M. Vespa, R. Dähn, E. Gallucci, D. Grolimund, E. Wieland, and A. M. Scheidegger

In situ microscale investigations of Ni uptake by cement reveal a highly heterogeneous distribution of Ni and a direct association to Ca–Si-containing cement phases.

■ **7710**

▶ **Using Nitrogen Isotope Fractionation To Assess Abiotic Reduction of Nitroaromatic Compounds**

Akané Hartenbach, Thomas B. Hofstetter, Michael Berg, Jakov Bolotin, and René P. Schwarzenbach

Substantial nitrogen isotope fractionation of four nitroaromatic compounds suggests that apparent kinetic isotope effects can be used to assess the fate of nitrogen-containing contaminants in subsurface environments.

■ **7717**

**Quantum Chemical Calculations of Sulfate Adsorption at the Al- and Fe-(Hydr)oxide-$H_2O$ Interface—Estimation of Gibbs Free Energies**

Kristian W. Paul, James D. Kubicki, and Donald L. Sparks

The Gibbs free energy of sulfate adsorption on variably charged Al- and Fe-(hydr)oxides is estimated with molecular orbital/density functional theory cluster calculations.

■ **7725**

**Excess Colloid Retention in Porous Media as a Function of Colloid Size, Fluid Velocity, and Grain Angularity**

Meiping Tong and William P. Johnson

Retention in flow stagnation zones in porous media in the presence of an energy barrier is an important removal mechanism for a wide range of colloid sizes.

■ **7732**

**Using Nitrogen and Carbon Dioxide Molecules To Probe Arsenic(V) Bioaccessibility in Soils**

Konstantinos C. Makris, Dibyendu Sarkar, Rupali Datta, Peter I. Ravikovitch, and Alexander V. Neimark

Soil As bioaccessibility is adequately described with a simple empirical model consisting of representative chemical (TOC) and physical (specific surface area) soil properties.

**7739**

**Model Bacterial Extracellular Polysaccharide Adsorption onto Silica and Alumina: Quartz Crystal Microbalance with Dissipation Monitoring of Dextran Adsorption**

Kideok D. Kwon, Hans Green, Patrik Bjöörn, and James D. Kubicki

A quartz crystal microbalance with dispersion is used to study adsorption of model bacterial polysaccharides onto silica and alumina; the ability to measure kinetics and nanoscale structure is demonstrated.

**7745**

**XAS and XMCD Evidence for Species-Dependent Partitioning of Arsenic during Microbial Reduction of Ferrihydrite to Magnetite**

V. S. Coker, A. G. Gault, C. I. Pearce, G. van der Laan, N. D. Telling, J. M. Charnock, D. A. Polya, and J. R. Lloyd

Synchrotron techniques (XAS and XMCD) are used to study the incorporation of arsenate into magnetite during the dissimilatory microbial reduction of ferrihydrite.

**7751**

**Quantifying the Availability of Clay Surfaces in Soils for Adsorption of Nitrocyanobenzene and Diuron**

Simone M. Charles, Hui Li, Brian J. Teppen, and Stephen A. Boyd

The availability of clay minerals in soil for adsorption of organic compounds is experimentally quantified and is linked to mineral surface coverage by soil organic matter.

■ **7757**

**Effect of Natural Organic Substances on the Surface and Adsorptive Properties of Environmental Black Carbon (Char): Attenuation of Surface Activity by Humic and Fulvic Acids**

Joseph J. Pignatello, Seokjoon Kwon, and Yufeung Lu

Loading of humic substances greatly reduces the $N_2$ BET surface area and presents competition for adsorption of organic compounds at external surfaces.

■ **7764**

**Methylmercury in Freshwater Fish Linked to Atmospheric Mercury Deposition**

Chad R. Hammerschmidt and William F. Fitzgerald

In the U.S., statewide average concentrations of methylmercury in wild populations of largemouth bass vary positively with wet atmospheric fluxes of mercury among many states.

■ **7771**

**Factors Affecting the Efficiency of Carbon Monoxide Photoproduction in the St. Lawrence Estuarine System (Canada)**

Yong Zhang, Huixiang Xie, and Guohua Chen

Water temperature and origin and light history of chromophoric dissolved organic matter affect the efficiency of carbon monoxide photoproduction in marine waters.

■ **7778**

**Assessment of Isotope Exchange Methodology To Determine the Sorption Coefficient and Isotopically Exchangeable Concentration of Selenium in Soils and Sediments**

Richard N. Collins, Ngoc D. Tran, Estelle Bakkaus, Laure Avoscan, and Barbara Gouget

The redox states of selenium, and their isotope self-exchange reactions, need to be identified when sorption coefficients and $E$ values are measured in soils and sediments.

■ **7784**

**Arsenate Sorption on Lithium/Aluminum Layered Double Hydroxide Intercalated by Chloride and on Gibbsite: Sorption Isotherms, Envelopes, and Spectroscopic Studies**

Yu Ting Liu, Ming Kuang Wang, Tsan Yao Chen, Po Neng Chiang, Pan Ming Huang, and Jhy Fu Lee

The sorption capacity of Li/Al LDH-Cl for arsenate is shown to be superior to that of $Al(OH)_3$, because it transforms the inert $Al(OH)_3$ surface into active sorption sites.

■ **7790**

**Wavelength Dependence of Fe(II) Photoformation in the Water-Soluble Fraction of Aerosols Collected in Okinawa, Japan**

Kouichirou Okada, Yukiko Kuroki, Yoshihide Nakama, Takemitsu Arakaki, and Akira Tanahara

Fe(II) photoformation in solutions of the water-soluble fraction of aerosols collected in Okinawa, Japan, shows wavelength dependency.

**7796**

**Novel Aerobic Perchloroethylene Degradation by the White-Rot Fungus *Trametes versicolor***

Ernest Marco-Urrea, Xavier Gabarrell, Montserrat Sarrà, Gloria Caminal, Teresa Vicent, and C. Adinarayana Reddy

The fungus *T. versicolor* can aerobically degrade perchloroethylene to trichloroacetic acid, and inhibitory experiments suggest that cytochrome P-450 is involved in the degradation.

## ENVIRONMENTAL MODELING

■ **7803**

### Source Apportionment of Molecular Markers and Organic Aerosol. 1. Polycyclic Aromatic Hydrocarbons and Methodology for Data Visualization

Allen L. Robinson, R. Subramanian, Neil M. Donahue, Anna Bernardo-Bricker, and Wolfgang F. Rogge

Mixing of emissions from different sources and photochemical aging on PAH concentrations is examined with a data visualization technique and chemical mass balance monitoring.

■ **7811**

### Source Apportionment of Molecular Markers and Organic Aerosol. 2. Biomass Smoke

Allen L. Robinson, R. Subramanian, Neil M. Donahue, Anna Bernardo-Bricker, and Wolfgang F. Rogge

Variability in source profiles and ambient biomass smoke marker concentrations creates uncertainty in chemical mass balance results.

■ **7820**

### Source Apportionment of Molecular Markers and Organic Aerosol. 3. Food Cooking Emissions

Allen L. Robinson, R. Subramanian, Neil M. Donahue, Anna Bernardo-Bricker, and Wolfgang F. Rogge

Ambient concentrations of cooking markers are strongly correlated, but inconsistencies between ambient data and source profiles create significant uncertainty in chemical mass balance results.

■ **7828**

### On-Road Heavy-Duty Diesel Particulate Matter Emissions Modeled Using Chassis Dynamometer Data

Tom Kear and D. A. Niemeier

Operational correction factors are estimated to adjust on-road heavy-duty diesel particle emission rates to reflect real-world driving conditions that are not captured with current driving cycles.

■ **7834**

### Vulnerability of Shallow Groundwater and Drinking-Water Wells to Nitrate in the United States

Bernard T. Nolan and Kerie J. Hitt

New national models predict nitrate concentration in shallow groundwater and in drinking-water wells.

■ **7841**

### Forecasting Acidification Effects Using a Bayesian Calibration and Uncertainty Propagation Approach

Thorjørn Larssen, Ragnar B. Huseby, Bernard J. Cosby, Gudmund Høst, Tore Høgåsen, and Magne Aldrin

A Bayesian approach is combined with a hydrogeochemical model (MAGIC) to calculate probability distributions for water quality and fish population health in the future with different scenarios of acid deposition.

■ **7848**

### Estimating Nutrients and Chlorophyll *a* Relationships in Finnish Lakes

Olli Malve and Song S. Qian

A hierarchical linear model that predicts the response of chlorophyll *a* to variations in lake total phosphorus and total nitrogen concentrations is fitted to a large cross-sectional data set from the Finnish Lake Monitoring Network.

## ENVIRONMENTAL MEASUREMENTS METHODS

■ **7854**

### Struggle for Quality in Determination of Perfluorinated Contaminants in Environmental and Human Samples

Stefan P. J. van Leeuwen, Anna Kärrman, Bert van Bavel, Jacob de Boer, and Gunilla Lindström

The first worldwide interlaboratory study on perfluorinated compounds shows that the analytical methodologies are not yet fully mastered.

■ **7861**

### Measurement of Dissolved $H_2$, $O_2$, and $CO_2$ in Groundwater Using Passive Samplers for Gas Chromatographic Analyses

B. P. Spalding and D. B. Watson

A short length of tubing attached to a syringe is adapted for passive sampling of dissolved gases in groundwater; this simplifies field collection and sample handling.

**7868**

### Cavity Ring-Down Spectroscopy of Ambient $NO_2$ with Quantification and Elimination of Interferences

James Hargrove, Liming Wang, Karen Muyskens, Mark Muyskens, David Medina, Susan Zaide, and Jingsong Zhang

Ambient measurement of $NO_2$ by cavity ring-down spectroscopy at 405 nm is examined and corrected for interferences with a $NO_2$ denuder.

■ **7874**

### Characterizing Dissolved and Particulate Phosphorus in Water with $^{31}P$ Nuclear Magnetic Resonance Spectroscopy

Barbara J. Cade-Menun, John A. Navaratnam, and Mark R. Walbridge

Dissolved and particulate phosphorus in 4-L river-water samples are characterized by solution $^{31}P$-NMR spectroscopy, and differences between river inlet and floodplain samples are detected.

## REMEDIATION AND CONTROL TECHNOLOGIES

**7881**

### Treatment of Odorous Sulphur Compounds by Chemical Scrubbing with Hydrogen Peroxide—Stabilisation of the Scrubbing Solution

Isabelle Charron, Annabelle Couvert, Alain Laplanche, Christophe Renner, Lucie Patria, and Benoît Requieme

Several chemical additives for the stabilization of hydrogen peroxide are tested.

**7886**

### The Fate of Fluorine and Chlorine during Thermal Treatment of Coals

Shaoqing Guo, Jianli Yang, and Zhenyu Liu

Fluorine and chlorine compounds released from coal processing are investigated for their toxicity to plants and animals as well as their contribution to equipment corrosion.

**7890**

### Collection of Ultrafine Diesel Particulate Matter (DPM) in Cylindrical Single-Stage Wet Electrostatic Precipitators

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

## SUSTAINABILITY ENGINEERING AND GREEN CHEMISTRY



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## ADDITIONS AND CORRECTIONS



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