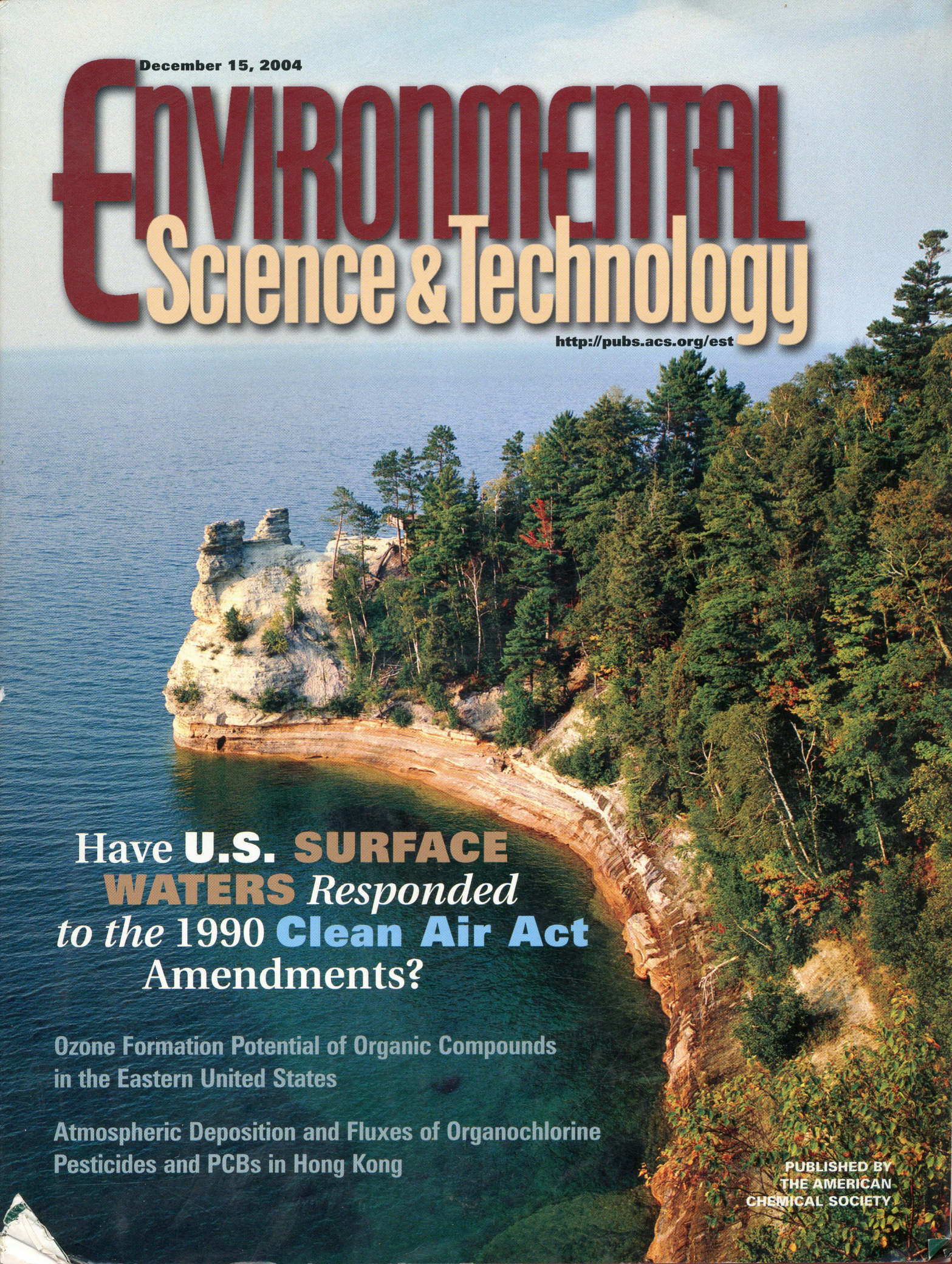


December 15, 2004

ENVIRONMENTAL Science & Technology

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Have **U.S. SURFACE
WATERS** *Responded*
to the 1990 **Clean Air Act**
Amendments?

Ozone Formation Potential of Organic Compounds
in the Eastern United States

Atmospheric Deposition and Fluxes of Organochlorine
Pesticides and PCBs in Hong Kong

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THE AMERICAN
CHEMICAL SOCIETY

Research

Policy Analysis

■ **6441**
Initial Public Perceptions of Deep Geological and Oceanic Disposal of Carbon Dioxide

Claire R. Palmgren, M. Granger Morgan, Wändi Bruine de Bruin, and David W. Keith
Likely public perceptions are assessed of technology to remove carbon dioxide in power plants and inject it into deep geological formations or the deep ocean.

Characterization of Natural and Affected Environments

6451
Comparison of Risk Assessment Methodologies for Exposure of Mink to PCBs on the Kalamazoo River, Michigan

Stephanie D. Millsap, Alan L. Blankenship, Patrick W. Bradley, Paul D. Jones, Denise Kay, Arianne Neigh, Cyrus Park, Karl D. Strause, Matthew J. Zwiernik, and John P. Giesy
An approach based on hepatic concentrations of PCBs and 2,3,7,8-tetrachlorodibenzo-*p*-dioxin equivalents is compared with one based on concentrations in the diet.

6460
Effects of Historical Lake Level and Land Use on Sediment and Phosphorus Accumulation Rates in Lake Kinneret

K. David Hambright, Werner Eckert, Peter R. Leavitt, and Claire L. Schelske
Sediment patterns suggest that hydrologic management of natural lakes can increase sedimentary nutrient flux when lake volume and water levels become more variable.

6468
Chemical Forms of Mercury and Cadmium Accumulated in Marine Mammals and Seabirds as Determined by XAFS Analysis

Teruko Arai, Tokutaka Ikemoto, Akiko Hokura, Yasuko Terada, Takashi Kunito, Shinsuke Tanabe, and Izumi Nakai
XAFS analysis discloses the existence of a mercury chalcogenide containing both Hg-Se and Hg-S bonds in black-footed albatross; this suggests a solid solution Hg(Se, S).

■ **6475**
Fluorinated Organic Compounds in an Eastern Arctic Marine Food Web

Gregg T. Tomy, Wes Budakowski, Thor Halldorson, Paul A. Helm, Gary A. Stern, Ken Friesen, Karen Pepper, Sheryl A. Tittlemier, and Aaron T. Fisk
PFOS is detected in all species analyzed, whereas PFOA is detected in fewer samples at generally smaller concentrations; zooplankton contains the greatest concentrations of PFOA.

6482
Characterization of Background Concentrations in Upper Manhattan, New York, Apartments for Select Contaminants Identified in World Trade Center Dust

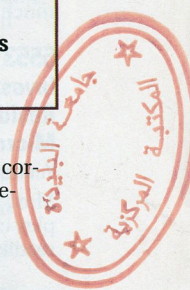
Kai M. Tang, Charles G. Nace, Jr., Carol L. Lynes, Mark A. Maddaloni, Dore LaPosta, and Kathleen C. Callahan
Results suggest probable levels of contaminants in Lower Manhattan residential buildings prior to the attack and will enhance the available database for characterizing indoor environments.

■ **6491**
Trends in Secondary Organic Aerosol at a Remote Site in Michigan's Upper Peninsula

Rebecca J. Sheesley, James J. Schauer, Erin Bean, and Donna Kenski

Notices to ES&T authors

1. Effective now, titles must be included in the Reference section of *ES&T* research papers.
2. Effective January 1, 2005, 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.



Distributions of particle-phase organic diacids are found to correlate with secondary organic aerosol and air-mass source regions at a remote site in the Great Lakes.

6501
Surfactants in Atmospheric Aerosols

Mohd Talib Latif and Peter Brimblecombe
Colorimetric methods show the ubiquitous presence of anionic surfactant on aerosols at concentrations of hundreds of pmol/m³.

6507
Plutonium from Global Fallout Recorded in an Ice Core from the Belukha Glacier, Siberian Altai

Susanne Olivier, Sixto Bajo, L. Keith Fifield, Heinz W. Gäggeler, Tatyana Papina, Peter H. Santschi, Ulrich Schotterer, Margit Schwikowski, and Lukas Wacker
Plutonium concentrations and ²⁴⁰Pu/²³⁹Pu isotopic ratios in an ice core indicate global stratospheric fallout as the plutonium source for the midlatitude region of Siberia.

6513
Atmospheric Deposition and Fluxes of Organochlorine Pesticides and Coplanar Polychlorinated Biphenyls in Aquatic Environments of Hong Kong, China

Hui Lam Wong, John P. Giesy, and Paul Kwan Sing Lam
The first comprehensive study of atmospheric deposition and fluxes of organochlorines and coplanar polychlorinated biphenyls in aquatic environments of Hong Kong, China, is described.

■ **6522**
Lead Isotopes in Lichen Transplants around a Cu Smelter in Russia Determined by MC-ICP-MS Reveal Transient Records of Multiple Sources

B. Spiro, D. J. Weiss, O. W. Purvis, I. Mikhailova, B. J. Williamson, B. J. Coles, and V. Udachin
Accurate lead isotope ratios in lichens resolve various sources of atmospheric deposition, including particles that are retained temporarily at steady state in extracellular surficial positions.

6529
Passive-Sampler-Derived Air Concentrations of Persistent Organic Pollutants on a North-South Transect in Chile

Karla Pozo, Tom Harner, Mahiba Shoeib, Roberto Urrutia, Ricardo Barra, Oscar Parra, and Silvano Focardi
Passive samplers reveal air concentrations of persistent organic pollutants in remote locations along a north-south transect in Chile.

6538
Isolating Isomers of Perfluorocarboxylates in Polar Bears (*Ursus maritimus*) from Two Geographical Locations

Amila O. De Silva and Scott A. Mabury
PFCA isomer profiles in polar-bear liver samples are dominated by the linear isomer; branched PFCA isomer composition varies with location.

■ Supporting Information is available free of charge via the Internet at <http://pubs.acs.org>.

6546

Watershed Land Use Is Strongly Linked to PCBs in White Perch in Chesapeake Bay Subestuaries

Ryan S. King, Joseph R. Beaman, Dennis F. Whigham, Anson H. Hines, Matthew E. Baker, and Donald E. Weller

The amount of watershed development near estuaries explains as much as 99% of the variance in total PCBs in white perch filets.

6553

Investigation of the Microcharacteristics of PM_{2.5} in Residual Oil Fly Ash by Analytical Transmission Electron Microscopy

Yuanzhi Chen, Naresh Shah, Frank E. Huggins, and Gerald P. Huffman

Most individual inorganic particles in ROFA PM_{2.5} exhibit complex chemistry. Composite particles typically exist in the form of readily soluble, potentially bioavailable multimetal sulfates.

Environmental Processes

6561

Formation of Metal-Arsenate Precipitates at the Goethite-Water Interface

Markus Gräfe, Maarten Nachtegaal, and Donald L. Sparks

Arsenate and zinc form a precipitate at the goethite-water interface at pH 7 under incremental, undersaturated concentrations.

6571

Stream-Subsurface Exchange of Zinc in the Presence of Silica and Kaolinite Colloids

Jianhong Ren and Aaron I. Packman

Laboratory experiments and numerical simulations are used to investigate multiphase contaminant transport behavior, namely the stream-subsurface exchange and immobilization of zinc in the presence of colloidal silica and kaolinite.

■ 6582

Particle-Phase Acidity and Oligomer Formation in Secondary Organic Aerosol

Song Gao, Nga L. Ng, Melita Keywood, Varuntida Varutbangkul, Roya Bahreini, Athanasios Nenes, Jiwen He, Kee Y. Yoo, J. L. Beauchamp, Robert P. Hodyss, Richard C. Flagan, and John H. Seinfeld

Oligomers may be ubiquitous aerosol components, and particle-phase acidity has a direct impact on the composition and yield of secondary organic aerosols.

6590

Phosphorus Immobilization in Micropores of Drinking-Water Treatment Residuals: Implications for Long-Term Stability

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

Chemical and solid-state evidence for hysteretic phosphorus sorption in micropores of drinking-water treatment residuals has favorable implications for long-term stability of phosphorus in WTR-amended soils.

6597

Lutetium Speciation and Toxicity in a Microbial Bioassay: Testing the Free-Ion Model for Lanthanides

Lennart Weltje, Lars R. C. W. Verhoof, Wilko Verweij, and Timo Hamers

The toxicity of trivalent lutetium to *Vibrio fischeri* agrees with the free-ion model.

6605

Ultraviolet Radiation Affects Emission of Ozone-Depleting Substances by Marine Macroalgae: Results from a Laboratory Incubation Study

Frank Laturnus, Teresia Svensson, Christian Wiencke, and Gunilla Öberg

Laboratory incubation studies reveal that elevated levels of UV radiation lead to an increase in the emission of reactive organic halogens by marine macroalgae.

6610

Sediment and Porewater Profiles and Fluxes of Mercury and Methylmercury in a Small Seepage Lake in Northern Minnesota

Neal A. Hines, Patrick L. Brezonik, and Daniel R. Engstrom

Total mercury and methylmercury are measured in sediment and sediment porewater of a small seepage lake; results show net demethylation in the sediment environment.

6618

Interaction of Inorganic Arsenic with Biogenic Manganese Oxide Produced by a Mn-Oxidizing Fungus, Strain KR21-2

Yukinori Tani, Naoyuki Miyata, Maiko Ohashi, Toshihiko Ohnuki, Haruhiko Seyama, Keisuke Iwahori, and Mitsuyuki Soma

Oxidation rate of As(III) and adsorption extent of As(V) by a biogenic manganese oxide are significantly influenced by Mn²⁺ bound to the oxide surface.

6625

Influence of Frozen Storage on Herbicide Degradation Capacity in Surface and Subsurface Sandy Soils

Sarah K. Mortensen and Carsten S. Jacobsen

Frozen storage of soil samples that are not normally subjected to freeze-thaw cycles is acceptable for the assessment of pesticide degradation.

■ 6633

Equilibrium Distribution of Polysulfide Ions in Aqueous Solutions at 25 °C: A New Approach for the Study of Polysulfides' Equilibria

Alexey Kamyshny, Jr., Anatoly Goifman, Jenny Gun, Dan Rizkov, and Ovidia Lev

An approach based on rapid, chemical derivatization in a single phase is introduced and used to determine the thermodynamics of inorganic polysulfides in aqueous solutions.

6645

Using ¹⁹F NMR Spectroscopy To Determine Trifluralin Binding to Soil

Mark Strynar, Jerzy Dec, Alan Benesi, A. Daniel Jones, Roderick A. Fry, and Jean-Marc Bollag

Reduction of trifluralin nitro groups and covalent binding of the resulting amino derivatives to soil organic matter are determined using ¹⁹F NMR.

6656

Formation of Studtite during the Oxidative Dissolution of UO₂ by Hydrogen Peroxide: An SFM Study

F. Clarens, J. de Pablo, I. Diez-Pérez, I. Casas, J. Giménez, and M. Rovira

The SFM technique is used to follow the precipitation of studtite (UO₄ · 4H₂O) during the oxidative dissolution of UO₂ by hydrogen peroxide.

■ 6662

Sorption-Controlled Degradation Kinetics of MCPA in Soil

Pia H. Jensen, Hans Chr. B. Hansen, Jim Rasmussen, and Ole S. Jacobsen

Mineralization rates of MCPA in sorbent-amended soil are strongly correlated with sorption strength of MCPA, and only the water-extractable MCPA is readily mineralized.

6669

MSWI Fly Ash Particle Analysis by Scanning Electron Microscopy-Energy Dispersive X-ray Spectroscopy

S. Gilardoni, P. Fermo, F. Cariati, V. Gianelle, D. Pitea, E. Collina, and M. Lasagni

The distribution of chlorine, copper, iron, and zinc on MSWI fly ash is investigated by electron microscopy/X-ray fluorescence spectroscopy.

■ 6676

Reductive Dechlorination of Carbon Tetrachloride in Aqueous Solutions Containing Ferrous and Copper Ions

R. A. Maithreepala and Ruy-an Doong

The reaction of Cu(II) with dissolved Fe(II) produces different morphologies of ferric oxides to accelerate the dechlorination rate of CCl_4 .

■ 6685

UV Photolysis of Trichloroethylene: Product Study and Kinetic Modeling

Ke Li, Mihaela I. Stefan, and John C. Crittenden

Trichloroethylene photolysis generates chloride ions and reaction intermediates such as formic, di- and monochloroacetic, and glyoxylic acids, and byproducts undergo further photolysis.

6694

Sorption and Desorption Behavior of Tributyltin with Natural Sediments

Edward D. Burton, Ian R. Phillips, and Darryl W. Hawker

Sorption and desorption of tributyltin to natural sediments is strongly influenced by pH and salinity; this behavior can be explained by consideration of aqueous TBT speciation.

6701

Diesel Bus Emissions Measured in a Tunnel Study

Milan Jamriska, Lidia Morawska, Steven Thomas, and Congrong He

Emission factors for particles, from road measurements at a tunnel's entrance and exit, are compared with dynamometer studies and literature emission factors.

6710

Characterizing the Metal Adsorption Capability of a Class F Coal Fly Ash

Jianmin Wang, Xinjun Teng, Hao Wang, and Heng Ban

Methods to determine the metal adsorption capacity and strength of fly ash are discussed, and mathematical models to quantify pH impact on metal adsorption are presented.

Environmental Modeling

■ 6716

Modeling the Effect of Algal Dynamics on Arsenic Speciation in Lake Biwa

Ferdi L. Hellweger and Upmanu Lal

The model reproduces both the observed ecology—including rapid uptake of phosphate by phytoplankton without immediate growth after lake overturn—and the observed arsenic speciation.

■ 6724

Consensus kNN QSAR: A Versatile Method for Predicting the Estrogenic Activity of Organic Compounds In Silico. A Comparative Study with Five Estrogen Receptors and a Large, Diverse Set of Ligands

Arja H. Asikainen, Juhani Ruuskanen, and Kari A. Tuppurainen

The ability of the consensus kNN QSAR method to predict estrogenic activity of organic molecules is demonstrated with different receptors and a set of ligands.

6730

Model Simulations of NO_x and Ultrafine Particles Close to a Swedish Highway

L. Gidhagen, C. Johansson, G. Omstedt, J. Langner, and G. Olivares

Coagulation matters little downwind of the highway, and high friction velocities enhance local deposition; beyond 10 m downwind, the removal rate is low and advected ultrafine particles are almost inert.

■ 6741

Optimization under Variability and Uncertainty: A Case Study for NO_x Emissions Control for a Gasification System

Jianjun Chen and H. Christopher Frey

Optimization methods under variability and uncertainty are proposed and demonstrated via application to NO_x emissions control for an IGCC system.

■ 6748

Ozone Formation Potential of Organic Compounds in the Eastern United States: A Comparison of Episodes, Inventories, and Domains

Amir Hakami, Michelle S. Bergin, and Armistead G. Russell

Relative impacts of various volatile organic compound emissions are quantified with a direct sensitivity analysis technique and may support possible reactivity-based regulations.

Environmental Measurements Methods

■ 6760

Statistical Method To Evaluate the Occurrence of PCB Transformations in River Sediments with Application to Hudson River Data

Sandra C. Karcher, Mitchell J. Small, and Jeanne M. VanBriesen

This study exploits the ratio relationship of PCB congeners in Aroclors to evaluate the likelihood of congener transformation and/or preferential congener transport in river sediments.

6767

Development of a DNA Microarray Chip for the Identification of Sludge Bacteria Using an Unsequenced Random Genomic DNA Hybridization Method

Byoung Chan Kim, Ji Hyun Park, and Man Bock Gu

A DNA chip with random genomic DNA probes can be used for a specific bacterial identification in activated sludge and other microbial community processes.

■ 6775

Development and Evaluation of Microarray-Based Whole-Genome Hybridization for Detection of Microorganisms within the Context of Environmental Applications

Liyou Wu, Dorothea K. Thompson, Xueduan Liu, Matthew W. Fields, Christopher E. Bagwell, James M. Tiedje, and Jizhong Zhou

A community genome array was evaluated and found to be a specific, sensitive, and quantitative tool for the species-level detection and identification of microorganisms in environmental samples.

■ 6783

Testing Groundwater for Arsenic in Bangladesh before Installing a Well

A. van Geen, T. Protus, Z. Cheng, A. A. Horneman, A. A. Seddique, M. A. Hoque, and K. M. Ahmed

A simple sampling device allows local teams of drillers in Bangladesh to target groundwater that is low in arsenic before installing a well.

■ 6790

Comparison of Two Field Sampling Procedures (En Core and Field Methanol Extraction) for Volatile Organic Compounds

Ann M. Vega, Vicki A. Lancaster, and Michael H. Roulter

The volatile organic compound concentrations of soil samples from field methanol extraction and En Core are statistically compared.

6795

Development of a Class-Specific ELISA for Sulfonylurea Herbicides (Sulfuron Screen)

Petra Degelmann, Jean Wenger, Reinhard Niessner, and Dietmar Knopp

A class-specific ELISA (sulfuron screen) is developed that can detect 16 sulfonylurea compounds at a concentration of 100 ppt or below in tap water and surface water.

6803

Anaerobic Reductive Dechlorination of 1-Chloro-1-fluoroethene To Track the Transformation of Vinyl Chloride

George Pon and Lewis Semprini

■ Supporting Information is available free of charge via the Internet at <http://pubs.acs.org>.

1-Chloro-1-fluoroethene can be used as a reactive tracer to track the anaerobic reductive dechlorination of vinyl chloride.

6809

Development and Application of a Mobile Laboratory for Measuring Emissions from Diesel Engines. 2. Sampling for Toxics and Particulate Matter

David R. Cocker III, Sandip D. Shah, Kent C. Johnson, Xiaona Zhu, J. Wayne Miller, and Joseph M. Norbeck

Emission rates for carbonyls, 1,3-butadiene, benzene, toluene, xylene, particulate matter, and elemental and organic carbon are reported for a vehicle transiting a major transportation corridor.

■ **6817**

Investigation of Conventional Membrane and Tangential Flow Ultrafiltration Artifacts and Their Application to the Characterization of Freshwater Colloids

Matthew A. Morrison and Gaboury Benoit

Effects of filtration technique and size cutoff on filtrate element concentrations and artifacts for natural freshwater samples are investigated using both membrane and tangential flow ultrafiltration.

6824

Balancing Measurement Uncertainty against Financial Benefits: Comparison of In Situ and Ex Situ Analysis of Contaminated Land

Paul D. Taylor, Michael H. Ramsey, and Philip J. Potts

In situ PXRF measurements of contamination generate higher uncertainty but are shown as more cost-effective than laboratory-based techniques when judged using the OCLI method.

Remediation and Control Technologies

■ **6832**

Antibiotics in the Environment: Occurrence in Italian STPs, Fate, and Preliminary Assessment on Algal Toxicity of Amoxicillin

Roberto Andreozzi, Vincenzo Caprio, Claudia Ciniglia, Marcella de Champdoré, Roberto Lo Giudice, Raffaele Marotta, and Ettore Zuccato

Abiotic and biotic transformations of amoxicillin in the aquatic environment are studied and lead to the assessment of kinetic parameters for direct solar photolysis and biodegradation.

6839

Adhesion Kinetics of Viable *Cryptosporidium parvum* Oocysts to Quartz Surfaces

Zachary A. Kuznar and Menachem Elimelech

Because of electrosteric repulsion, the deposition rate of *C. parvum* oocysts on quartz surfaces is markedly lower in monovalent electrolyte solution compared with divalent salt.

6846

Use of Polymer Mats in Series for Sequential Reactive Barrier Remediation of Ammonium-Contaminated Groundwater: Field Evaluation

B. M. Patterson, M. E. Grassi, B. S. Robertson, G. B. Davis, A. J. Smith, and A. J. McKinley

This study evaluates a pilot-scale field trial using in situ polymer mats, installed as permeable reactive barriers, to induce sequential bioremediation of ammonium-contaminated groundwater.

■ **6855**

Transformation of Herbicide Propachlor by an Agrochemical Thiourea

Wei Zheng, Scott R. Yates, Sharon K. Papiernik, and Mingxin Guo

The transformation of the herbicide Propachlor with nitrification inhibitor thiourea is investigated to explore the feasibility of the chemical remediation on reducing pesticide contaminants.

6861

Decomposition of the Polycyclic Nitramine Explosive, CL-20, by Fe⁰

Vimal K. Balakrishnan, Fanny Monteil-Rivera, Annamaria Halasz, Aurelian Corbeanu, and Jalal Hawari

Zerovalent iron degrades CL-20 in anaerobic aqueous suspensions to produce formic acid, glyoxal, glycolic acid, nitrite, ammonia, nitrous oxide, and nitrogen.

6867

Novel Dry-Desulfurization Process Using Ca(OH)₂/Fly Ash Sorbent in a Circulating Fluidized Bed

Norihiko Matsushima, Yan Li, Masateru Nishioka, Masayoshi Sadakata, Haiying Qi, and Xuchang Xu

The dry-desulfurization process removes SO₂ in flue gas with a high efficiency under dry conditions; CaSO₄, the primary byproduct, can be used for soil amendment.

6875

Kinetics and Mechanism of Photoactivated Periodate Reaction with 4-Chlorophenol in Acidic Solution

Liang-Hiong Chia, Xueming Tang, and Linda K. Weavers

Under low irradiation intensities, at 266 nm, and at pH 3, 4-CP degrades by pseudo-first-order reaction kinetics; O^{(3)P} and IO₃[•] are suspected reactive species.

■ **6881**

Kinetics of Haloacetic Acid Reactions with Fe(0)

Li Zhang, William A. Arnold, and Raymond M. Hozalski

A kinetic model for reactions of haloacetic acids with Fe(0) is developed; the potential importance of such reactions in drinking-water distribution systems is estimated.

6890

Caged Multiwalled Carbon Nanotubes as the Adsorbents for Affinity-Based Elimination of Ionic Dyes

Bunshi Fugetsu, Shuya Satoh, Toshikazu Shiba, Taeko Mizutani, Yong-Bo Lin, Norifumi Terui, Yoshinobu Nodasaka, Katsushi Sasa, Kiyoko Shimizu, Tsukasa Akasaka, Masanobu Shindoh, Ken-ichiro Shibata, Atsuro Yokoyama, Masanobu Mori, Kazuhiko Tanaka, Yoshinori Sato, Kazuyuki Tohji, Shunitz Tanaka, Norio Nishi, and Fumio Watari

Caged MWCNTs, obtained by immobilizing the nanotubes in cross-linked alginate, demonstrate great potential for elimination of ionic dyes from contaminated water.

Sustainability Engineering and Green Chemistry

6897

Exploration of the Role of Heat Activation in Enhancing Serpentine Carbon Sequestration Reactions

Michael J. McKelvy, Andrew V. G. Chizmeshya, Jason Diefenbacher, Hamdallah Béarat, and George Wolf

The role of heat activation and the associated metaserpentine formation in enhancing serpentine carbon sequestration reaction processes is explored.

Correspondence/Rebuttal

6904

Comment on "Simulating the Influence of Snow on the Fate of Organic Compounds"

Daniel L. Carlson and Ronald A. Hites

6905

Response to Comment on "Simulating the Influence of Snow on the Fate of Organic Compounds"

Gillian L. Daly and Frank Wania

6907

Author Index to Volume 38, 2004

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