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Challenges in **ECOTOXICOLOGY**

Looking beyond Kyoto

Subways grind out a dose of fine metals

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Critical Review

■ 657

System Boundary Selection in Life Cycle Inventories Using Hybrid Approaches

Sangwon Suh, Manfred Lenzen, Graham J. Treloar, Hiroki Hondo, Arpad Horvath, Gjaltp Huppel, Olivier Jolliet, Uwe Klann, Wolfram Krewitt, Yuichi Moriguchi, Jesper Munksgaard, and Gregory Norris

System boundary issues in life cycle assessment are discussed, and hybrid approaches as methods for resolving the boundary selection problem are highlighted.

Characterization of Natural and Affected Environments

665

History and Environmental Impact of Mining Activity in Celtic Aeduan Territory Recorded in a Peat Bog (Morvan, France)

F. Monna, C. Petit, J.-P. Guillaumet, I. Jouffroy-Bapicot, C. Blanchot, J. Dominik, R. Losno, H. Richard, J. Lévêque, and C. Chateau

The geochemical and pollen analysis of a peat core collected around Bibracte demonstrates early mining operations and the significant environmental impact of our ancestors' industrial activities.

674

Direct Speciation of Phosphorus in Alum-Amended Poultry Litter: Solid-State ^{31}P NMR Investigation

Stefan Hunger, Herman Cho, James T. Sims, and Donald L. Sparks

Solid-state ^{31}P NMR spectroscopy is used to identify and quantify phosphate species in unamended and alum-amended poultry litter.

682

Human-Cell Mutagens in Respirable Airborne Particles in the Northeastern United States. 1. Mutagenicity of Fractionated Samples

Daniel U. Pedersen, John L. Durant, Bruce W. Penman, Charles L. Crespi, Harold F. Hemond, Arthur L. Lafleur, and Glen R. Cass

Semipolar fractions were most mutagenic at all five sites studied and were twofold more mutagenic at upstate New York sites than at Massachusetts sites.

690

Influence of Altitude and Age in the Accumulation of Organochlorine Compounds in Fish from High Mountain Lakes

Ingrid Vives, Joan O. Grimalt, Jordi Catalan, Björn O. Rosseland, and Rick W. Battarbee

Organochlorine compounds in fish from high mountain lakes depend on fish age and lake altitude due to condensation at low temperatures, depleted metabolism, and respiration.

699

PBDEs in the Atmosphere of Three Locations in Western Europe

Robert G. M. Lee, Gareth O. Thomas, and Kevin C. Jones

Atmospheric concentrations of PBDEs are measured at three locations in Western Europe, and controlling factors are investigated.

707

Reconstruction of a Century of Airborne Asbestos Concentrations

James S. Webber, Kenneth W. Jackson, Pravin P. Parekh, Richard F. Bopp

Airborne asbestos concentrations are reconstructed for the entire 20th century through a combination of paleolimnological methods, particle separation techniques, and analytical transmission electron microscopy.

■ 715

Observations on Historical, Contemporary, and Natural PCDD/Fs

Nicholas J. L. Green, Ashraf Hassanin, A. E. Johnston, and Kevin C. Jones

Evidence is provided for the widespread occurrence of PCDD/Fs in the environment prior to 1900 as well as for a complex array of sources and environmental transformation processes.

■ 724

Spatial Distribution of Polybrominated Diphenyl Ethers in Southern Ontario as Measured in Indoor and Outdoor Window Organic Films

Craig M. Butt, Miriam L. Diamond, Jennifer Truong, Michael G. Ikononou, and Arnout F. H. ter Schure

PBDE concentrations and profiles are reported in outdoor and indoor window organic films along an urban-rural transect in southern Ontario, Canada.

■ 732

Elevated Airborne Exposures of Teenagers to Manganese, Chromium, and Iron from Steel Dust and New York City's Subway System

Steven N. Chillrud, David Epstein, James M. Ross, Sonja N. Sax, Dee Pederson, John D. Spengler, and Patrick L. Kinney

Steel dust generated in the New York City subway appears to control airborne exposures to iron, manganese, and chromium among subway-riding adolescents in this study.

■ 738

PBDEs in European Background Soils: Levels and Factors Controlling Their Distribution

Ashraf Hassanin, Knut Breivik, Sandra N. Meijer, Eiliv Steinnes, Gareth O. Thomas, and Kevin C. Jones

PBDE levels match those of PCBs in European background soils, and the mixture implies little weathering of the penta product.

Environmental Processes

746

Modeling the Oxidative Capacity of the Atmosphere of the South Coast Air Basin of California. 1. Ozone Formation Metrics

Robert J. Griffin, Meghan K. Revelle, and Donald Dabdub

Variables include the O_3 production rate, production efficiency, and total reactivity (the sum of the reactivity of CO and all organic gases reacting with the hydroxyl radical).

753

Modeling the Oxidative Capacity of the Atmosphere of the South Coast Air Basin of California. 2. HO_x Radical Production

Robert J. Griffin

With the exceptions of the ALK-O and H_2O_2 -hv routes, all pathways investigated are significant sources of HO_x production under the scenarios presented.

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

► This issue contains a news story about this research.

758

Biotransformation of *N*-Ethyl Perfluorooctanesulfonamide by Rainbow Trout (*Onchorhynchus mykiss*)

Liver Microsomes

Gregg T. Tomy, Sheryl A. Tittlemier, Vince P. Palace, Wes R. Budakowski, Eric Braekevelt, Lyndon Brinkworth, and Ken Friesen

N-EtPFOSA is biotransformed to PFOSA and PFOS by rainbow trout liver microsomes.

763

Adsorption and Transport of Gas-Phase Naphthalene on Micron-Size Fog Droplets in Air

Suresh Raja and Kalliat T. Valsaraj

Small droplet diameter, decreased temperature, and the presence of dissolved surface-active material may enhance the uptake of hydrophobic organic compounds into fog droplets.

769

Role of *Leptothrix discophora* in Mediating Metal Uptake in the Filter-Feeding Bivalve *Mytilus trossulus* (*edulis*)

Joline R. Widmeyer, E. Daryl Crozier, Margo M. Moore, Astrid Jurgensen, and Leah I. Bendell-Young

M. trossulus ingests higher-quality bacterial food sources at an increased rate, resulting in higher uptake of high-quality food-associated Cd and Pb.

775

Characterization of Metal–Cyanobacteria Sorption Reactions: A Combined Macroscopic and Infrared Spectroscopic Investigation

Nathan Yee, Liane G. Benning, Vernon R. Phoenix, and F. Grant Ferris

This study combines macroscopic and infrared spectroscopic techniques to investigate the functional group chemistry and metal-binding properties of cyanobacterial surfaces.

783

Cl K-edge X-ray Spectroscopic Investigation of Enzymatic Formation of Organochlorines in Weathering Plant Material

Rachel G. Reina, Alessandra C. Leri, and Satish C. B. Myneni

Organochlorines are produced from reactions of Cl⁻ in *Sequoia sempervirens* needles in the presence of a chloroperoxidase released by common fungi in the environment.

790

Fate and Transport of Testosterone in Agricultural Soils

Francis X. M. Casey, Heldur Hakk, Jiří Šimůnek, and Gerald L. Larsen

Batch sorption experiments, column transport experiments, and modeling are used to study the sorption, mobility, and transformation of testosterone in agricultural soils.

■ 799

Reactivity of Fe(II)-Bearing Minerals toward Reductive Transformation of Organic Contaminants

Martin Elsner, René P. Schwarzenbach, and Stefan B. Haderlein

Surface-area-normalized rate constants for dehalogenation and nitroaryl reduction by surface-bound Fe(II) at different minerals varied by orders of magnitude and followed this general trend: siderite < iron oxides < iron sulfides.

808

Uptake and Elimination Routes of Inorganic Mercury and Methylmercury in *Daphnia magna*

Martin T. K. Tsui and Wen-Xiong Wang

Dietary exposure and water exposure are both important in bioaccumulation, whereas maternal transfer plays a role in the process of elimination of Hg(II) and MeHg.

817

Effects of Dissolved Carbonate on Arsenate Adsorption and Surface Speciation at the Hematite–Water Interface

Yuji Arai, D. L. Sparks, and J. A. Davis

The retention of inner-sphere bidentate arsenate surface species at the hematite (α -Fe₂O₃)–water interface is kinetically enhanced and/or suppressed by dissolved bicarbonate ions.

825

Formation of PBCDD and PBCDF during Flue Gas Cooling

Gunilla Söderström and Stellan Marklund

The chlorine:bromine ratio for PBCDD/F in flue gas increases as the temperature decreases.

831

Photolysis of Chloral under Atmospheric Conditions

John C. Wenger, Stéphane Le Calvé, Howard W. Sidebottom, Klaus Wirtz, Montserrat Martín Reviejo, and James A. Franklin

Photolysis by sunlight is shown to be the dominant atmospheric loss process for chloral (CCl₃CHO) and produces phosgene (CCl₂O), CO, and Cl atoms.

Environmental Modeling

■ 838

Screening Analysis of Human Pharmaceutical Compounds in U.S. Surface Waters

Paul D. Anderson, Vincent J. D'Aco, Peter Shanahan, Steven C. Chapra, Mary E. Buzby, Virginia L. Cunningham, Beth M. DuPlessie, Eileen P. Hayes, Frank J. Mastrocco, Neil J. Parke, John C. Rader, John H. Samuelian, and Bradley W. Schwab

Using a mass balance approach, the Pharmaceutical Assessment and Transport Evaluation model predicts screening-level concentrations of active pharmaceutical ingredients and related compounds.

■ 850

Global Analysis of the Riverine Transport of ⁹⁰Sr and ¹³⁷Cs

Jim T. Smith, Simon M. Wright, Matthew A. Cross, Luigi Monte, Anatoly V. Kudelsky, Ritva Saxén, Sergei M. Vakulovsky, and David N. Timms

Global-scale soil and land use data sets are used to predict the riverine transport of radiocesium and radiostrontium in European and Asian catchments.

Environmental Measurements Methods

858

Method Development for the Determination of Diacetyl and Acetoin at a Microwave Popcorn Plant

Stephanie M. Pendergrass

A sampling and analytical methodology for diacetyl and acetoin exposures in a microwave popcorn plant is described.

862

Determination of Airborne Carbonyls: Comparison of a Thermal Desorption/GC Method with the Standard DNPH/HPLC Method

Steven Sai Hang Ho and Jian Zhen Yu

The thermal desorption/GC method provides better peak separation and more sensitive and specific detection through the use of a mass spectrometric detector.