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Toxic Effects of CONTAMINANTS in Polar Marine Environments

Formation of Chloroform and Chlorinated Organics by Free-Chlorine-Mediated Oxidation of Triclosan

Microbial Phenazine Production
Enhances Electron Transfer in Biofuel Cells

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Research

Policy Analysis

2913

A Predictive Approach to Nutrient Criteria

K. H. Reckhow, G. B. Arhonditsis, M. A. Kenney, L. Hauser, J. Tribo, C. Wu, K. J. Elcock, L. J. Steinberg, C. A. Stow, and S. J. McBride Expert elicitation and structural-equation modeling are used to identify predictive nutrient criteria and then express the result as a probability of designated-use attainment.

2920

Probabilistic Ecological Risk Assessment of 1,2,4-Trichlorobenzene at a Former Industrial Contaminated Site

Marcello Zolezzi, Claudia Cattaneo, and José V. Tarazona The probabilistic approach represents a useful tool for refining site-specific ecological risk assessments of contaminated sites.

Characterization of Natural and Affected Environments

2927

Retrospective Search for Evidence of the 1957 Windscale Fire in NE Ireland Using ¹²⁹I and Other Long-Lived Nuclides

D. Gallagher, E. J. McGee, P. I. Mitchell, V. Alfimov, A. Aldahan, and G. Possnert

The recent history of radioisotope fallout from anthropogenic sources is recorded in high-resolution lake cores from County Down, Northern Ireland.

2936

Tollbooth Workers and Mobile Source-Related Hazardous Air Pollutants: How Protective Is the Indoor Environment?

Amir Sapkota, D'Ann Williams, and Timothy J. Buckley Considerable protection is afforded to workers by their indoor environment, most likely by the positive-pressure-control ventilation system in the facility.

2944

Fluorotelomer Carboxylic Acids and PFOS in Rainwater from an Urban Center in Canada

Mark Loewen, Thor Halldorson, Feiyue Wang, and Gregg Tomy Saturated and unsaturated telomer acids are present at low nanogram-per-liter concentrations in rainwater samples collected in Winnipeg, Canada.

2952

Gas-Phase Concentrations of Current-Use Pesticides in Iowa

Aaron M. Peck and Keri C. Hornbuckle

Current-use pesticides were measured in air at urban, rural, and suburban sites in eastern Iowa during 2000–2002.

2960

Some Pesticides Occurrence in Air and Precipitation in Québec, Canada

Fabien Aulagnier and Laurier Poissant

Several OC pesticides measured in the atmosphere and in precipitation at agricultural and remote locations in Québec are examined for their sources, fate, and seasonal pattern.

2968

Measuring and Predicting Environmental Concentrations of Pesticides in Air after Application to Paddy Water Systems

Federico Ferrari, Dimitrios G. Karpouzas, Marco Trevisan, and Ettore Capri Volatilization of pesticides from paddy water systems could be a significant dissipation process, and it should be considered in the pesticide risk-assessment process.

2976

Contribution of Biomass Burning to Atmospheric Polycyclic Aromatic Hydrocarbons at Three European Background Sites

Manolis Mandalakis, Örjan Gustafsson, Tomas Alsberg, Anna-Lena Egebäck, Christopher M. Reddy, Li Xu, Jana Klanova, Ivan Holoubek, and Euripides G. Stephanou

Radiocarbon source apportionment suggests that biomass burning contributes 50% of the atmospheric PAHs at a Swedish background site but only 10% to corresponding sites in southern Europe.

2983

Concentration and Distribution of Heavy Metals in Urban Airborne Particulate Matter in Frankfurt am Main, Germany

Fathi Zereini, Friedrich Alt, Jürgen Messerschmidt, Clare Wiseman, Ingo Feldmann, Alex von Bohlen, Jürgen Müller, Karlheinz Liebl, and Wilhelm Püttmann

The highest airborne heavy-metal concentrations occur near the main, heavily trafficked streets; this suggests that motor vehicles are the source of the emissions.

2990

Hydroxylated and Methoxylated Brominated Diphenyl Ethers in the Red Algae *Ceramium tenuicorne* and Blue Mussels from the Baltic Sea

Anna Malmvärn, Göran Marsh, Lena Kautsky, Maria Athanasiadou, Åke Bergman, and Lillemor Asplund

Hydroxylated and methoxylated polybrominated diphenyl ethers are identified by comparison with authentic synthesized standards in algae and mussels from the Baltic Sea.

2998

Rapid Changes in PCB and OC Pesticide Concentrations in Arctic Snow

B. M. J. Herbert, C. J. Halsall, S. Villa, K. C. Jones, and R. Kallenborn A rapid decline in surface snow concentrations is observed for both PCB and OC pesticides; this decline is related to snow aging and changes in snow density.

3006

Posidonia oceanica as a Historical Monitor Device of Lead Concentration in Marine Environment

L. Tranchina, S. Miccichè, A. Bartolotta, M. Brai, and R. N. Mantegna We show that the scales of *Posidonia oceanica* are a reliable biomonitor for measuring the level of lead pollution in a coastal marine environment.

3013

Stereoisomer Composition of the Chiral UV Filter 4-Methylbenzylidene Camphor in Environmental Samples

Hans-Rudolf Buser, Markus D. Müller, Marianne E. Balmer, Thomas Poiger, and Ignaz J. Buerge

The initially racemic composition of 4-MBC in personal-care products is modified after release to the aquatic environment by enantioselective processes in lakes and fish.

Environmental Processes

3020

Experimental and Computational Studies of the Gas-Phase Reaction of Halon 1211 with Hydrogen

Hai Yu, Eric M. Kennedy, Md. Azhar Uddin, Simon P. Sullivan, and Boqdan Z. Dlugogorski

A kinetic reaction scheme involving 90 species and 430 reaction steps is developed and used to model the halon 1211 hydrodehalogenation reaction.

3029

Conservation of Cancer Genes in the Marine Invertebrate Mytilus edulis

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

Corina M. Ciocan and Jeanette M. Rotchell

The conservation of cancer genes ras and p53 in Mytilus edulis is described.

3034

Methylmercury in Mosquitoes Related to Atmospheric Mercury Deposition and Contamination

Chad R. Hammerschmidt and William F. Fitzgerald Mosquitoes may be a sensitive indicator of food-web methylmercury accumulation and atmospheric mercury deposition.

3040

Cadmium Uptake by a Green Alga Can Be Predicted by Equilibrium Modelling

Heliana Kola and Kevin J. Wilkinson

Cadmium biouptake by two strains of *Chlamydomonas reinhardtii* is quantitatively predicted by $[Cd^{2+}]$ over a wide range of pH, $[Ca^{2+}]$, and concentrations of other competing ions.

3048

Extended X-ray Absorption Fine Structure Spectroscopy Evidence for the Complexation of Cadmium by Reduced Sulfur Groups in Natural Organic Matter

Torbjörn Karlsson, Per Persson, and Ulf Skyllberg Reduced sulfur groups in natural organic matter are involved in the complexation of cadmium.

3056

Modeling Cadmium Exchange by an Aquatic Moss (Fontinalis dalecarlica)

Louis Croisetière, Landis Hare, André Tessier, and Sophie Duchesne A two-compartment model successfully describes cadmium uptake and loss by the aquatic moss *Fontinalis dalecarlica*.

3061

Arsenic Mobilization through Microbially Mediated Deflocculation of Ferrihydrite

Christopher J. Tadanier, Madeline E. Schreiber, and Jonathan W. Roller Bioreduction of As-bearing ferrihydrite by *Geobacter metalli-reducens* leads to mineral transformation, which causes surface charge alteration, subsequent deflocculation of micrometer-sized ferrihydrite aggregates, and formation of nanometer-sized colloids.

3069

Simultaneous Utilization of Acetate and Hydrogen by Geobacter sulfurreducens and Implications for Use of Hydrogen as an Indicator of Redox Conditions

Derick G. Brown, John Komlos, and Peter R. Jaffé Multisubstrate kinetics of $\rm H_2$ and acetate use under iron-reducing conditions are presented, along with the implications of these kinetics on aqueous $\rm H_2$ concentrations.

3077

Thermal Growth and Decomposition of Methylnaphthalenes

Jun Yang and Mingming Lu

Product formation mechanisms from the combustion of 1- and 2-methylnaphthalenes—the main alkylated aromatic components in diesel fuels—are experimentally investigated.

3083

Recovery of Chlorine-Exposed Escherichia coli in Estuarine Microcosms

Carl H. Bolster, Jonathan M. Bromley, and Stephen H. Jones
The inoculation of estuarine water microcosms containing
chlorine-injured *E. coli* resulted in significant increases in the
concentrations of culturable cells over a three-day period.

3090

In Vitro Assessment of Modes of Toxic Action of Pharmaceuticals in Aquatic Life

Beate I. Escher, Nadine Bramaz, Rik I. L. Eggen, and Manuela Richter

An in vitro test battery provides preliminary hazard assessment and classification of the mode of toxic action for pharmaceuticals in the aquatic environment.

3101

Black Carbon and Ecological Factors Affect In Situ Biota to Sediment Accumulation Factors for Hydrophobic Organic Compounds in Flood Plain Lakes

Caroline T. A. Moermond, John J. G. Zwolsman, and Albert A. Koelmans Measured and modeled results show that both black carbon and ecological factors explain the variation of in situ BSAFs for hydrophobic organic compounds.

3110

Cloud Point Extraction of Direct Yellow

Elzbieta Tatara, Katarzyna Materna, Achim Schaadt, Hans-Jörg Bart, and Jan Szymanowski

The cloud-point phenomenon of nonionic surfactants induces the separation of an aqueous phase and a surfactant-rich phase that concentrates the dye.

3116

Effect of Chemical Speciation on Toxicity of Mercury to Escherichia coli Biofilms and Planktonic Cells

Isaac Najera, Chu-Ching Lin, Golenaz Adeli Kohbodi, and Jennifer A. Jay The relationship between Hg uptake and speciation along a chloride gradient is similar in biofilm and planktonic cultures of *E. coli*.

3121

Photochemical Oscillation of Fe(II)/Fe(III) Ratio Induced by Periodic Flux of Dissolved Organic Matter

Wenjing Song, Wanhong Ma, Jiahai Ma, Chuncheng Chen, and Jincai Zhao

Variations of iron species in the presence of different dissolved organic matter were examined in UV-irradiated aqueous solutions.

3128

Hydrolysis of Environmental Contaminants as an Experimental Tool for Indication of Their Persistency

Sara Rahm, Nicholas Green, Jessica Norrgran, and Åke Bergman To improve understanding of persistency, a method is described for estimating the relative susceptibility of some potential environmental pollutants to hydrolysis reactions.

3134

Sorption and Related Properties of the Swine Antibiotic Carbadox and Associated N-Oxide Reduced Metabolites

Troy J. Strock, Stephen A. Sassman, and Linda S. Lee Sorption of the swine antibacterial drug carbadox and its metabolites is influenced by organic-matter content, clay type, and the inorganic cations that are present.

3143

Impact of the Hydrocarbon to NO_x Ratio on Secondary Organic Aerosol Formation

Chen Song, Kwangsam Na, and David R. Cocker, III Lower NO_x levels generate considerably more secondary organic aerosol mass than higher levels, when reacted m-xylene is held constant.

3150

Influence of Smectite Hydration and Swelling on Atrazine Sorption Behavior

Mark A. Chappell, David A. Laird, Michael L. Thompson, Hui Li, Brian J. Teppen, Vaneet Aggarwal, Cliff T. Johnston, and Stephen A. Boyd The atrazine sorption behavior of a smectite is significantly influenced by crystalline swelling, which controls the hydration status of the smectite interlayers.

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

3157

Kinetic Desorption and Sorption of U(VI) during Reactive Transport in a Contaminated Hanford Sediment

Nikolla P. Qafoku, John M. Zachara, Chongxuan Liu, Paul L. Gassman, Odeta S. Qafoku, and Steven C. Smith

Laboratory experiments find strong kinetic effects for U(VI) desorption and sorption; these results suggest that the release and transport of the contaminant in the field are probably kinetically controlled.

3166

Comparison of Copper Speciation in Estuarine Water Measured Using Analytical Voltammetry and Supported Liquid Membrane Techniques

Kuria Ndungu, Matthew P. Hurst, and Kenneth W. Bruland A supported liquid membrane incorporating a carboxylic polyether ionophore, lasalocid, as a membrane carrier is used to measure copper speciation in estuarine water.

3176

► Formation of Chloroform and Chlorinated Organics by Free-Chlorine-Mediated Oxidation of Triclosan

Krista L. Rule, Virginia R. Ebbett, and Peter J. Vikesland Triclosan readily reacts with free chlorine under drinking-water conditions to produce chlorinated phenols and chloroform.

Environmental Modeling

3186

Illustrating Sensitivity and Uncertainty in Environmental Fate Models Using Partitioning Maps

Torsten Meyer, Frank Wania, and Knut Breivik Maps of environmental parameter sensitivity from multimedia, mass-balance model results provide valuable insights into organic contaminant fate and model behavior.

3197

Retrospective Analyses and Future Predictions of Snowmelt-Induced Acidification: Example from a Heavily Impacted Stream in the Czech Republic

H. Laudon, J. Hruška, S. Köhler, and P. Krám

A model is presented for hindcast and forecast of transient short-term acidification, and it is applied to the Lysina catchment in the Czech Republic.

3203

Indoor Sorption of Surrogates for Sarin and Related Nerve Agents

Brett C. Singer, Alfred T. Hodgson, Hugo Destaillats, Toshifumi Hotchi, Kenneth L. Revzan, and Richard G. Sextro

Indoor environment sorption models are presented for nerve agents, with parameter values determined experimentally using surrogates; because of sorption, sheltering indoors substantially reduces toxic load.

3215

Modeling the Influence of Decomposing Organic Solids on Sulfate Reduction Rates for Iron Precipitation

Paulo S. Hemsi, Charles D. Shackelford, and Linda A. Figueroa Modeling illustrates the influence of the type of kinetics used to describe the decomposition of organic solids on metal precipitation in sulfate-reducing systems.

3226

Critical Body Residues Linked to Octanol—Water Partitioning, Organism Composition, and LC₅₀ QSARs: Meta-Analysis and Model

A. Jan Hendriks, Theo P. Traas, and Mark A. J. Huijbregts Accumulation models for lipid and nonlipid phases for various modes of action and species groups are used to link LC_{50} QSARs to lethal body burdens.

3237

Predicting Methyl *tert*-Butyl Ether, *tert*-Butyl Formate, and *tert*-Butyl Alcohol Levels in the Environment Using the Fugacity Approach

Hans Peter H. Arp, Kathrin Fenner, and Torsten C. Schmidt A multimedia transformation model, parameterized according to known sensitivities, successfully predicts environmental concentrations of MTBE and its transformation products TBF and TBA in Europe.

3245

Optimization-Based Source Apportionment of PM_{2.5} Incorporating Gas-to-Particle Ratios

Amit Marmur, Alper Unal, James A. Mulholland, and Armistead G.

Use of gas-phase species has been found useful in deriving more reliable source contributions of $PM_{2.5}$ in Atlanta, Ga., and in reducing collinearity between sources.

3255

Effect of Declining Lake Base Cation Concentration on Freshwater Critical Load Calculations

Shaun A. Watmough, Julian Aherne, and Peter J. Dillon
The impact of soil acidification on the determination of critical loads of acidity for freshwaters is presented.

Environmental Measurements Methods

3261

A Field Comparison of Volatile Organic Compound Measurements Using Passive Organic Vapor Monitors and Stainless Steel Canisters

Gregory C. Pratt, Don Bock, Thomas H. Stock, Maria Morandi, John L. Adgate, Gurumurthy Ramachandran, Steven J. Mongin, and Ken Sexton The methods are in agreement for some compounds but not all, with the observed differences similar across measurement sites, seasons, and meteorological variables.

3269

Estimating Ground-Level PM_{2.5} in the Eastern United States Using Satellite Remote Sensing

Yang Liu, Jeremy A. Sarnat, Vasu Kilaru, Daniel J. Jacob, and Petros Koutrakis

Aerosol optical thickness measurements derived from satellite remote sensors may provide a cost-effective and supplemental source of information for determining ground-level $\rm PM_{2.5}.$

3279

Evaluation of Methods To Obtain Geosorbent Fractions Enriched in Carbonaceous Materials That Affect Hydrophobic Organic Chemical Sorption

Sangjo Jeong and Charles J. Werth

Chemical and thermal treatments used to obtain carbonaceous material enrichments of geosorbents are applied to a char, two soots, and a humic acid.

3289

New Method for Assimilable Organic Carbon Determination Using Flow-Cytometric Enumeration and a Natural Microbial Consortium as Inoculum

Frederik A. Hammes and Thomas Egli

A new method based on flow-cytometric cell enumeration is presented. It allows quick and realistic determination of assimilable organic carbon by natural microbial consortia.

3295

Field-Flow Fractionation—Inductively Coupled Plasma Mass Spectrometry: An Alternative Approach to Investigate Metal—Humic Substances Interaction

Atitaya Siripinyanond, Sumattana Worapanyanond, and Juwadee Shiowatana

Field-flow fractionation—inductively coupled plasma mass spectrometry is a useful hyphenated technique for investigating metal distributions in different-sizedfractions of humic aggregates.

3302

A New In Situ Method to Analyze Mineral Particle Reactions in Soils

Andreas Birkefeld, Rainer Schulin, and Bernd Nowack

A new experimental in situ method is used to analyze the dissolution and phase transformation of small mineral particles in soils under field conditions.

Remediation and Control Technologies

3308

Sorption Enhancement of Aromatic Sulfonates onto an Aminated Hyper-Cross-Linked Polymer

Bingcai Pan, Quanxing Zhang, Fanwei Meng, Xiaotiao Li, Xiao Zhang, Jianzhong Zheng, Weiming Zhang, Bingjun Pan, and Jinlong Chen Amacroreticular resin adsorbent, CHA-101, is aminated by dimethylamine to obtain a novel sorbent named M-101.

3314

Preparation and Characterization of a New Class of Starch-Stabilized Bimetallic Nanoparticles for Degradation of Chlorinated Hydrocarbons in Water

Feng He and Dongye Zhao

Starched palladized iron (Fe–Pd) nanoparticles prepared with a water-soluble starch are less agglomerating and more reactive than nonstarched nanoparticles.

3321

Chromium Release from Waste Incineration Air-Pollution-Control Residues

T. Astrup, C. Rosenblad, S. Trapp, and T. H. Christensen Al(0), which is present in the residues, controls chromium leaching by reducing Cr(VI); exposure to oxygen depletes the reduction capacity of Al(0) and causes increased chromium leaching.

3330

Pot and Field Studies on Bioremediation of *p*-Nitrophenol Contaminated Soil Using *Arthrobacter protophormiae* RKJ100

Sumeet Labana, Gunjan Pandey, Debarati Paul, Narinder K. Sharma, Aparaiita Basu, and Rakesh K. Jain

This study describes the successful bioremediation of soil contaminated with PNP in pot and field conditions using *Arthrobacter protophormiae* RKJ100 immobilized on the carrier material, corncob powder.

3338

Inactivation of Microorganisms Using Electrostatic Fields

Maosheng Yao, Gediminas Mainelis, and Hey Reoun An

Nonpulsed electrostatic fields can inactivate sensitive microorganisms residing on nonconductive surfaces, if the proper combination of field strength and exposure time is selected.

3345

Primary Measures for Reduction of PCDD/F in Co-Combustion of Lignite Coal and Waste: Effect of Various Inhibitors

Marchela E. Pandelova, Dieter Lenoir, Antonius Kettrup, and Karl-Werner Schramm

Inexpensive and nontoxic $(NH_4)_2SO_4$ and $(NH_4)_2S_2O_3$ are effective inhibitors of PCCD/F formation in flue gases, suppressing formation by >98%.

3351

Fate of Steroid Estrogens in Australian Inland and Coastal Wastewater Treatment Plants

Olga Braga, George A. Smythe, Andrea I. Schäfer, and Andrew J. Feitz

Steroid estrogens are not removed during enhanced primary treatment, and a large fraction remains attached to particles, with implications for the receiving marine environment.

3359

Thermal Treatment of Metal-Enriched Biomass Produced from Heavy Metal Phytoextraction

Catherine Keller, Christian Ludwig, Frédéric Davoli, and Jörg Wochele Experiments in a laboratory-scale reactor show that incineration is a viable option for the treatment of the heavy-metalenriched plants produced by phytoextraction.

3368

Controlled Release of Nitrate and Sulfate to Enhance Anaerobic Bioremediation of Phenanthrene in Marine Sediments

Yinjie J. Tang, Shelly Carpenter, Jody Deming, and Barbara Krieger-Brockett

The enhanced rates of microbial anaerobic phenanthrene degradation when controlled-release nitrocellulose and $CaSO_4$ are placed at depth in marine sediments are measured and interpreted.

3374

Removal of PAH Compounds from Liquid Fuels by Pd Catalysts

B. Pawelec, J. M. Campos-Martin, E. Cano-Serrano, R. M. Navarro, S. Thomas, and J. L. G. Fierro

Palladium catalysts supported on γ -alumina, amorphous silica—alumina, and zeolite β are prepared and evaluated for use in reducing PAHs in diesel fuel.

3382

Experimental Study of Water and Salt Fluxes through Reverse Osmosis Membranes

Wenwen Zhou and Lianfa Song

Water and salt fluxes through reverse osmosis membranes are experimentally investigated, and more appropriate transport equations are proposed.

3388

Sonochemical Decomposition of Perfluorooctane Sulfonate and Perfluorooctanoic Acid

Hiroshi Moriwaki, Youichi Takagi, Masanobu Tanaka, Kenshiro Tsuruho, Kenji Okitsu, and Yasuaki Maeda

A novel method, sonication, has been developed for the efficient decomposition of perfluorooctane sulfonate and perfluoroctanoic acid.

3393

Predicting Adsorption Isotherms for Aqueous Organic Micropollutants from Activated Carbon and Pollutant Properties

Lei Li, Patricia A. Quinlivan, and Detlef R. U. Knappe

Water affinity coefficients, which are correlated with adsorbent hydrophilicity, are combined with the Polanyi–Dubinin–Manes model to predict the adsorption of organic contaminants in aqueous solution by activated carbons.

Sustainability Engineering and Green Chemistry

3401

► Microbial Phenazine Production Enhances Electron Transfer in Biofuel Cells

Korneel Rabaey, Nico Boon, Monica Höfte, and Willy Verstraete Bacteria produce and/or use redox shuttles, thereby enhancing electron transfer in microbial fuel cells.

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