July 15, 2008

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The Challenges of RECYCLING POLYSTYRENE

How Effective Is Contaminated-Sediment Dredging?

An Improved Method To Assess Potential POPs

PUBLISHED BY THE AMERICAN CHEMICAL SOCIETY

Research

CHARACTERIZATION OF NATURAL AND AFFECTED ENVIRONMENTS

F-M-COLUMN

5049

Visible Light-Induced Plasmid DNA Damage Catalyzed by a CdSe/ZnS-Photosensitized Nano-TiO₂ Film

Xin-Cheng Shen, Zhi-Ling Zhang, Bo Zhou, Jun Peng, Min Xie, Min Zhang, and Dai-Wen Pang*

 $\mbox{CdSe/ZnS-photosensitized nano-TiO}_2$ films are of good photocatalytic ability to damage DNA and living bacteria under visible light.

5055

Occurrence of Two Genotypes of Tetracycline (TC) Resistance Gene tet(M) in the TC-Resistant Bacteria in Marine Sediments of Japan

M. Habibur Rahman, Lisa Nonaka, Ryosuke Tago, and Satoru Suzuki* tet(M) in marine sediment is investigated.

5062

The Influence of the Pre-Oxidation of Natural Organic Matter on the Formation of *N*-Nitrosodimethylamine (NDMA)

Zhuo Chen* and Richard L. Valentine*

NDMA formation from chloramination of NOM may be significantly reduced by a variety of preoxidants in proportional to the reduction in SUVA that also occurs as a consequence of these treatments.

5068

Characteristics of Particulate Carbon Emissions from Real-World Chinese Coal Combustion

Yuanxun Zhang, James Jay Schauer, Yuanhang Zhang, Limin Zeng, Yongjie Wei, Yuan Liu, and Min Shao*

Characterization of the emissions of the carbonaceous aerosols and molecular markers from real-world Chinese industrial and residential combustion of wood.

5074

Indoor Levels of Polycyclic Aromatic Hydrocarbons in Homes with or without Wood Burning for Heating

Pernilla Gustafson,* Conny Östman, and Gerd Sällsten

Domestic wood burning for space heating or pleasure increases indoor levels of many polycyclic aromatic hydrocarbons.

ENVIRONMENTAL PROCESSES

5081

Ozonolysis of eta-Pinene: Temperature Dependence of Secondary Organic Aerosol Mass Fraction

Ravikant Pathak, Neil M. Donahue, and Spyros N. Pandis*

Measurements of the formation of organic particulate matter during the atmospheric oxidation of one of the major biogenic hydrocarbons.

5087

Seasonal and Diurnal Variation of PM_{2.5} Apparent Particle Density in Urban Air in Augsburg, Germany

Mike Pitz,* Otmar Schmid, Joachim Heinrich, Wolfram Birmili, Jürgen Maguhn, Ralf Zimmermann, H.-Erich Wichmann, Annette Peters, and Josef Cyrys Apparent particle density of urban $PM_{2.5}$ shows pronounced seasonal and diurnal variation and strong correlations to standard particulate and meteorological parameters.

5094

Combining Spectroscopic and Potentiometric Approaches to Characterize Competitive Binding to Humic Substances

Laura Marang, Pascal E. Reiller, Sascha Eidner, Michael U. Kumke, and Marc F. Benedetti *

Competitive binding between a rare earth analogue and divalent cations onto humic substances reveals different binding sites for the rare earth elements.

5099

Dehalococcoides' Gene Transcripts As Quantitative Bioindicators of Tetrachloroethene, Trichloroethene, and cis-1,2-Dichloroethene Dehalorespiration Rates

Brian G. Rahm and Ruth E. Richardson*

This study explores the relationship between transcript abundance and respiration rate in tetrachloroethene-, trichloroethene-, and *cis*-1,2-dichloroethene-fed pseudosteady-state mixed cultures containing *Dehalococcoides ethenogenes*.

5106

Difference of Toxicity and Accumulation of Methylated and Inorganic Arsenic in Arsenic-Hyperaccumulating and -Hypertolerant Plants

Ze-Chun Huang, Tong-Bin Chen,* Mei Lei, Ying-Ru Liu, and Tian-Dou Hu Arsenic reduction, demethylation, toxicity, accumulation, and translocation in As-hyperaccumulating and -hypertolerant plants were compared using the XANES method.

5112

Combined Gel Probes for the In Situ Determination of Dissolved Reactive Phosphorus in Porewaters and Characterization of Sediment Reactivity

Phil Monbet,* Ian D. McKelvie, and Paul. J. Worsfold

Diffusive gel probes (DGT and DET) are used in a back-to-back configuration to investigate phosphorus dynamics in eutrophic coastal lagoon sediments.

5118

Mercury in Southeastern U.S. Riverine Fish Populations Linked to Water Body Type

Andrew L. Rypel, D. Albrey Arrington, and Robert H. Findlay*

Mercury in fishes is 3-fold higher in an unregulated Alabama river vs a nearby regulated river; this pattern is consistent across southeastern coastal plain rivers.

5125

Dissolved Gaseous Mercury Concentrations and Mercury Volatilization in a Frozen Freshwater Fluvial Lake

N. J. O'Driscoll,* L. Poissant, J. Canário, and D. R. S. Lean

Mercury inputs from both sediment diffusion and melting snow and ice explain the lack of correlation between dissolved gaseous mercury and mercury volatilization in a frozen lake.

5131

Fate of Tetracycline Resistance Genes in Aquatic Systems: Migration from the Water Column to Peripheral Biofilms

Christina A. Engemann, Patricia L. Keen, Charles W. Knapp, Kenneth J. Hall, and David W. Graham*

Most anthropogenic antibiotic resistance genes released into water disappear prior to reaching peripheral compartments; however, gene migration still occurs into biofilms and should be considered in future gene-fate models.

5137

Transitional Adsorption and Partition of Nonpolar and Polar Aromatic Contaminants by Biochars of Pine Needles with Different Pyrolytic Temperatures

Baoliang Chen,* Dandan Zhou, and Lizhong Zhu

The quantitative contributions of adsorption and partition of biochars are determined by the relative carbonized and noncarbonized fractions and their surface and bulk properties.

5144

The Internal Distribution of Nickel and Thallium in Two Freshwater Invertebrates and its Relevance to Trophic Transfer

Julie Dumas and Landis Hare*

Thallium and nickel are efficiently transferred from prey to predator, and transfer efficiency is related to subcellular metal distributions in prey.

5150

Reduction of Oxidized Mercury Species by Dicarboxylic Acids (C_2-C_4) : Kinetic and Product Studies

Lin Si and Parisa A. Ariya*

The kinetic data and product identification are obtained for the reduction of Hg^{II} by dicarboxylic acids (C_2 – C_4), of which the tentative mechanism is proposed.

5156

Do Ponds Cause Arsenic-Pollution of Groundwater in the Bengal Basin? An Answer from West Bengal

S. Sengupta, J. M. McArthur,* A. Sarkar, M. J. Leng, P. Ravenscroft, R. J. Howarth, and D. M. Banerjee

Conservative (δ^{18} O, δ^{2} H, K), and other tracers (Ca, Mg) of recharge in the Bengal Basin show that pond water drives neither FeOOH-reduction nor arsenic pollution.

5165

Catalytic Wet Air Oxidation of Aniline with Nanocasted Mn—Ce-Oxide Catalyst

R. Levi, M. Milman, M. V. Landau,* A. Brenner, and M. Herskowitz

Stable performance was observed in CWAO of acidified aniline (HCl/aniline = 1.2) in a trickle-bed reactor with nanocasted Mn–Ce-oxide catalyst yielding complete/90% aniline/TOC conversions.

■ 5171

Spatial and Seasonal Trends in Biogenic Secondary Organic Aerosol Tracers and Water-Soluble Organic Carbon in the Southeastern United States

Xiang Ding, Mei Zheng,* Liping Yu, Xiaolu Zhang, Rodney J. Weber, Bo Yan, Armistead G. Russell, Eric S. Edgerton, and Xinming Wang

Spatial and seasonal variations of isoprene and pinene SOA tracers and WSOC are investigated using one-year period samples collected at four CACHE (carbonaceous aerosol characterization experiment) sites.

5177

Laboratory Measurements of the Heterogeneous Oxidation of Condensed-Phase Organic Molecular Makers for Meat Cooking Emissions

Emily A. Weitkamp, Kara E. Huff Hartz, Amy M. Sage, Neil M. Donahue, and Allen L. Robinson*

Molecular markers for meat cooking oxidize rapidly in complex mixtures, and create large biases in source apportionment estimates for fine particulate matter.

ENVIRONMENTAL MODELING

5183

Modeling Dynamic Exchange of Gaseous Elemental Mercury at Polar Sunrise

Ashu P. Dastoor,* Didier Davignon, Nicolas Theys, Michel Van Roozendael, Alexandra Steffen, and Parisa A. Ariya

This study describes development of an atmospheric mercury model to simulate the springtime dynamic mercury cycling in the Polar Regions.

5189

How Do the Partitioning Properties of Polyhalogenated POPs Change When Chlorine Is Replaced with Bromine?

Tomasz Puzyn,* Noriyuki Suzuki, and Maciej Haranczyk

Computational study on the effect of replacement of chlorine with bromine on partition coefficients of persistent organic pollutants and its environmental consequences.

5196

Atmospheric Transport and Outflow of Polycyclic Aromatic Hydrocarbons from China

Chang Lang, Shu Tao,* Wenxin Liu, Yanxu Zhang, and Staci Simonich PAH outflow from China accounts for 7.1% of the total local emission and is under strong influence of regional climate

5202

conditions.

Screening Chemicals for the Potential to be Persistent Organic Pollutants: A Case Study of Arctic Contaminants

Trevor N. Brown and Frank Wania*

A highly selective screening method identifies 120 chemicals with partitioning, persistence, or structural attributes as well as production volumes that flag them as potential Arctic contaminants.

5210

Quantitative Structure—Property Relationships for Predicting Metal Binding by Organic Ligands

Stephen E. Cabaniss

Predictions of metal—organic complexation constants using only elemental and functional group composition have typical errors of 1 log unit for seven metals.

ENVIRONMENTAL MEASUREMENTS METHODS

5217

Determination of Primary, Secondary, and Tertiary Amines in Air by Direct or Diffusion Sampling Followed by Determination with Liquid Chromatography and Tandem Mass Spectrometry

Michael Rampfl,* Stefan Mair, Florian Mayer, Klaus Sedlbauer, Klaus Breuer, and Reinhard Niessner

The paper describes methods for direct and diffusive sampling and LC-MS/MS analysis of primary, secondary, and tertiary amines in material exhalation and ambient air samples.

5223

Effects of Sampling Artifacts on Occupational Samples of Diesel Particulate Matter

James Noll* and M. Eileen Birch

Correction for organic carbon sampling artifacts associated with quartz fiber filter collection of diesel particle matter in occupational setttings is examined.

5229

Real-Time PCR Detection and Quantification of Nine Potential Sources of Fecal Contamination by Analysis of Mitochondrial Cytochrome *b* Targets

William B. Schill* and Melvin V. Mathes

We describe quantitative polymerase chain reaction assays to determine mitochondrial DNA concentrations of nine vertebrate species and detect fecal contamination in environmental waters.

5235

An Empirical Approach to Estimating Detection Limits Using Collocated Data

Nicole P. Hyslop* and Warren H. White

Whole system detection limits are derived from XRF measurements using routine quality assurance data from two national $PM_{2.5}$ monitoring networks and IUPAC guidance.

5241

Experimental Investigation of the Rising Behavior of CO₂ Droplets in Seawater under Hydrate-Forming Conditions

Nikolaus K. Bigalke,* Gregor Rehder, and Giselher Gust

Experimentally determined rise velocities of both hydrate coated and pure liquid CO_2 droplets in pressurized seawater are reported and used to evaluate recent model parametrizations.

REMEDIATION AND CONTROL TECHNOLOGIES

5247

Heavy Metal Capture and Accumulation in Bioretention Media

Houng Li and Allen P. Davis*

Heavy metal accumulation profiles in bioretention media show a high surface accumulation, significantly decreasing with media depth.

5254

Persistence of Pathogenic Prion Protein during Simulated Wastewater Treatment Processes

Glen T. Hinckley, Christopher J. Johnson, Kurt H. Jacobson, Christian Bartholomay, Katherine D. McMahon, Debbie McKenzie, Judd M. Aiken, and Joel A. Pedersen*

The disease-associated form of the prion protein partitions to activated sludge solids and survives simulated mesophilic anaerobic sludge digestion.

5260

Quantification of Functional Groups and Modeling of Their Ionization Behavior in the Active Layer of FT30 Reverse Osmosis Membrane

Orlando Coronell, Benito J. Mariñas,* Xijing Zhang, and David G. Cahill Carboxylic and amine groups in the active layer of FT30 RO

membrane are characterized by Rutherford Backscattering spectrometry using silver and tungstate ions as probes.

5267

A Plate Produced by Nonmetallic Materials of Pulverized Waste Printed Circuit Boards

Jie Guo, Bin Cao, Jiuyong Guo, and Zhenming Xu*

A new method for resource utilization of nonmetallic materials reclaimed from waste printed circuit boards attains significant environmental benefits.

5272

Electrostatic Separation for Recovering Metals and Nonmetals from Waste Printed Circuit Board: Problems and Improvements

Jiang Wu, Jia Li, and Zhenming Xu*

This study reports problems and improvements in electrostatic separation of waste printed circuit boards using a roll-type separator.

5277

Transformation of Oxidation Products and Reduction of Estrogenic Activity of 17β -Estradiol by a Heterogeneous Photo-Fenton Reaction

Yaping Zhao,* Jiangyong Hu,* and Wei Jin

The reduction of 17β -estradiol with a relative estrogenicity and its degradation pathway by α -FeOOHR photocatalysis are investigated.

5285

Reactive Tracer Tests To Predict Dense Nonaqueous Phase Liquid Dissolution Dynamics in Laboratory Flow Chambers

X. Chen and J. W. Jawitz*

A single measureable parameter, reactive travel time variance, can be measured from tracer tests and then used to predict contaminant dissolution.

5292

Nanofiltration for Trace Organic Contaminant Removal: Structure, Solution, and Membrane Fouling Effects on the Rejection of Perfluorochemicals

Eva Steinle-Darling and Martin Reinhard*

The rejection of perfluorochemicals by NF membranes is generally effective, but can be decreased by lowered pH, membrane fouling, or increased membrane affinity (i.e., sorption).

5298

Determining Optimal Operation Parameters for Reducing PCDD/F Emissions (I-TEQ values) from the Iron Ore Sintering Process by Using the Taguchi Experimental Design

Yu-Cheng Chen, Perng-Jy Tsai,* and Jin-Luh Mou

The Taguchi experimental design is used to identify the optimal operating condition, and it provides useful approaches for reducing PCDD/Fs formations during the iron ore sintering process.

5304

Development of Silica/Vanadia/Titania Catalysts for Removal of Elemental Mercury from Coal-Combustion Flue Gas

Ying Li, Patrick D. Murphy, Chang-Yu Wu,* Kevin W. Powers, and Jean-Claude J. Bonzongo

Enhancement in elemental mercury removal from simulated coal-combustion flue gas is achieved through optimizing the composition and microstructures of synthesized silica/vanadia/titania catalysts.

5310

Affinity of Functional Groups for Membrane Surfaces: Implications for Physically Irreversible Fouling

Hiroshi Yamamura, Katsuki Kimura,* Takaharu Okajima, Hiroshi Tokumoto, and Yoshimasa Watanabe

The affinity of carbohydrate-like substances to two different microfiltration membranes is investigated by atomic force microscopy and functionally modified microspheres.

SUSTAINABILITY ENGINEERING AND GREEN CHEMISTRY

5316

Reactivity Enhancement of 2-Propanol Photocatalysis on SO_4^{2-}/TiO_2 : Insights from Solid-State NMR Spectroscopy

Hailu Zhang, Huaguang Yu, Anmin Zheng, Shenhui Li, Wanling Shen, and Feng Deng^*

Photocatalytic activity toward 2-propanol is remarkably enhanced on sulfated TiO_2 due to the preferential formation of Ti-bound 2-propoxy species.

5322

Optimal Control Theory for Sustainable Environmental Management

Yogendra Shastri, Urmila Diwekar,* and Heriberto Cabezas

Systems theory approach can successfully be used to understand dynamic interactions and develop management policy guidelines for complex ecosystem models to target sustainability.

5329

Potential for Carbon Adsorption on Concrete: Surface XPS Analyses

Liv M. Haselbach* and Shuguo Ma

XPS analyses indicate that carbonate species adsorbed on hydrated cement surfaces exceed calcination stoichiometry, important for understanding carbon sequestration processes in concrete.

ECOTOXICOLOGY AND HUMAN ENVIRONMENTAL HEALTH

5335

Acute Enhancement of Synaptic Transmission and Chronic Inhibition of Synaptogenesis Induced by Perfluorooctane Sulfonate through Mediation of Voltage-Dependent Calcium Channel

Chun-yang Liao, Xiang-yao Li, Bei Wu, Shumin Duan,* and Gui-bin Jiang*

Emerging pollutant perfluorooctane sulfonate produces evident excitotoxicity mediated by voltage-dependent calcium channel and inhibits neurite outgrowth and synaptogenesis in cultured rat hippocampal neurons.

5342

XAS Study of Arsenic Coordination in *Euglena gracilis* Exposed to Arsenite

Jennyfer Miot,* Guillaume Morin, Fériel Skouri-Panet, Céline Férard, Emmanuel Aubry, Joël Briand, Yuheng Wang, Georges Ona-Nguema, François Guyot, and Gordon E. Brown

X-ray absorption spectroscopy shows the key role of sulfur ligands for arsenite detoxification in the green alga *Euglena gracilis*.

5348

Indirect Evidence of Transposon-Mediated Selection of Antibiotic Resistance Genes in Aquatic Systems at Low-Level Oxytetracycline Exposures

Charles W. Knapp,* Christina A. Engemann, Mark L. Hanson, Patricia L. Keen, Kenneth J. Hall, and David W. Graham

Pseudochronic, subinhibitory oxytetracycline levels have environmental consequences on surface water quality and antibiotic resistance gene abundances in an outdoor mesocosm experiment.

5354

Natural Arsenic Contaminated Diets Perturb Reproduction in Fish

David Boyle, Kevin V. Brix, Heidi Amlund, Anne-Katrine Lundebye, Christer Hogstrand, and Nic R. Bury*

Zebrafish fed the polychaete *Nereis diversicolor* collected from a metal-impacted estuary accumulated arsenic and showed signs of impaired reproduction.

5361

Use of Newborn Screening Program Blood Spots for Exposure Assessment: Declining Levels of Perfluorinated Compounds in New York State Infants

Henry M. Spliethoff,* Lin Tao, Shannon M. Shaver, Kenneth M. Aldous, Kenneth A. Pass, Kurunthachalam Kannan, and George A. Eadon

Analysis of perfluorinated compounds in archived Newborn Screening Program blood spots demonstrates that exposures have been declining.

5368

High Accumulation of Perfluorooctane Sulfonate (PFOS) in Marine Tucuxi Dolphins (*Sotalia guianensis*) from the Brazilian Coast

Paulo R. Dorneles,* José Lailson-Brito, Alexandre F. Azevedo, Johan Meyer, Lara G. Vidal, Ana B. Fragoso, João P. Torres, Olaf Malm, Ronny Blust, and Krishna Das

Perfluorooctane sulfonate concentrations in marine tucuxi dolphins from Guanabara Bay, Rio de Janeiro state, Brazil are among the highest detected to date in cetaceans.

CORRESPONDENCE AND REBUTTAL

5374

Comment on "Avoidance of Aluminum Toxicity in Freshwater Snails Involves Intracellular Silicon—Aluminum Biointeraction"

Christopher Exley

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Response to Comment on "Avoidance of Aluminum Toxicity in Freshwater Snails Involves Intracellular Silicon—Aluminum Biointeraction"

Catherine R. McCrohan, Keith N. White, Rachel C. Walton, Andrew P. Brown, Ravin Jugdaohsingh, and Jonathan J. Powell

5377

Comment on "Factors Affecting the Yield of Oxidants from the Reaction of Nanoparticulate Zero-Valent Iron and Oxygen"

Jin Jiang, Su-Yan Pang, and Jun Ma

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Response to Comment on "Factors Affecting the Yield of Oxidants from the Reaction of Nanoparticulate Zero-Valent Iron and Oxygen"

Christina R. Keenan and David L. Sedlak

Supporting information is available free at http://pubs.acs.org/est.This research is highlighted in the News and Features section.