

May 15, 2008

ENVIRONMENTAL Science & Technology

<http://pubs.acs.org/est>



Interfacial Chemistry in Indoor Environments

Food Miles and the Climate
Impacts of Food Choices

Global Arsenic Contamination
in Groundwater

PUBLISHED BY
THE AMERICAN
CHEMICAL SOCIETY

POLICY ANALYSIS

■ 3501

National-Level Infrastructure and Economic Effects of Switchgrass Cofiring with Coal in Existing Power Plants for Carbon Mitigation

William R. Morrow,* W. Michael Griffin, and H. Scott Matthews

Based on a national-level linear programming methodology, incremental switchgrass and coal cofiring "cost of carbon mitigation" curves are presented along with regionally specific cofiring costs and policy issues.

■ 3508

Food-Miles and the Relative Climate Impacts of Food Choices in the United States

Christopher L. Weber* and H. Scott Matthews

The climate impacts of food choice in the United States are analyzed and the impacts from life-cycle transportation and life-cycle production are compared.

CHARACTERIZATION OF NATURAL AND AFFECTED ENVIRONMENTS

3514

Alkali Element Uptake in Otoliths: A Link Between the Environment and Otolith Microchemistry

Lisa A. Friedrich* and Norman M. Halden

A suite of alkali elements detected in otoliths is suggested to be linked to the local geology of the environment.

■ 3519

Use of Terrestrial Based Lipids in Aquaculture Feeds and the Effects on Flesh Organohalogen and Fatty Acid Concentrations in Farmed Atlantic Salmon

Erin N. Friesen, Michael G. Ikonou,* Dave A. Higgs, Keng Pee Ang, and Cory Dubetz

New aquafeeds with higher terrestrial lipid inclusion quantities lower persistent organic pollutant levels in farmed Atlantic salmon flesh to levels seen in wild Pacific salmon.

■ 3524

Source Apportionment and Spatial Distributions of Coarse Particles During the Regional Air Pollution Study

Injo Hwang, Philip K. Hopke,* and Joseph P. Pinto

Coarse particle composition data from 10 sites across St. Louis analyzed for source apportionments demonstrate heterogeneity of exposure across the region.

■ 3531

Ecological Factors Affecting Nitrate Concentrations in a Phreatic Desert Aquifer in Northwestern China

John B. Gates,* John Karl Böhlke, and W. Mike Edmunds

Isotopic data indicate local variation in the sources and cycling of nitrate in shallow groundwater in arid northwestern China.

■ 3538

Perfluorinated Surfactants in Surface, Subsurface Water and Microlayer from Dalian Coastal Waters in China

Xiaodong Ju, Yihe Jin,* Kazuaki Sasaki, and Norimitsu Saito

PFOA and PFOS are enriched significantly in coastal sea microlayer, and this has implications for designing measurement techniques, understanding their distribution, and sea spray-mediated transport.

ENVIRONMENTAL PROCESSES

■ 3543

Mobilization, Adsorption, and Bioavailability of Pt and Pd in Coastal Sediments: The Role of the Polychaete, *Arenicola marina*

Ben French and Andrew Turner*

Arenicola marina exert a significant impact on the biogeochemical behavior of platinum and palladium added to coastal sediments.

3550

Atmospheric SO₂ Emissions Since the Late 1800s Change Organic Sulfur Forms in Humic Substance Extracts of Soils

Johannes Lehmann,* Dawit Solomon, Fang-Jie Zhao, and Steve P. McGrath

Anthropogenic SO₂ emissions change the forms of organic S in humic substances extracts of soil, but decreasing emissions only lead to recovery after a lag period of almost decades.

3556

Coupled Effect of Chemotaxis and Growth on Microbial Distributions in Organic-Amended Aquifer Sediments: Observations from Laboratory and Field Studies

Meng Wang, Roseanne M. Ford,* and Ronald W. Harvey

Bacterial migration and distribution under the coupled effect of chemotaxis and growth from a consumable model contaminant were studied by applying a filter-chamber.

■ 3563

Kinetics of Microbial and Chemical Reduction of Humic Substances: Implications for Electron Shuttling

Jie Jiang and Andreas Kappler*

Quantification of kinetics of chemical and microbial redox reactions of humic substances and minimum concentrations of humic substances necessary for electron shuttling are investigated.

■ 3570

Degradation of Synthetic Androgens 17 α - and 17 β -Trenbolone and Trenbolone in Agricultural Soils

Bushra Khan, Linda S. Lee,* and Stephen A. Sassman

Aerobic degradation rates of 17 α - and 17 β -trenbolone to trenbolone are similar and inversely proportional to the log of the applied androgen concentration.

■ 3575

Oxidation State and Size of Fe Controlled by Organic Matter in Natural Waters

John W. Gaffney, Keith N. White, and Stephen Boulton*

Comparison between laboratory simulation and field survey indicates that natural organic matter controls the size and oxidation state of Fe in natural waters.

■ 3582

Stoichiometry of Ozonation of Environmentally Relevant Olefins in Saturated Hydrocarbon Solvents

Anthony L. Gomez, Tanza L. Lewis, Stacy A. Wilkinson, and Sergey A. Nizkorodov*

Ozone displays an unconventional reaction stoichiometry in oxidation of dilute solutions of unsaturated organics.

■ 3588

Transport and Retention of Nanoscale C₆₀ Aggregates in Water-Saturated Porous Media

Yonggang Wang, Yusong Li, John D. Fortner, Joseph B. Hughes, Linda M. Abriola, and Kurt D. Pennell*

Transport and retention of nC₆₀ aggregates are measured in water-saturated porous media and simulated using a mathematical model that incorporates attachment kinetics and a limiting retention capacity.

■ 3595

XANES—EXAFS Analysis of Se Solid-Phase Reaction Products Formed upon Contacting Se(IV) with FeS₂ and FeS

E. Breynaert, C. Bruggeman, and A. Maes*

Formation of Se⁰ and FeSe_x after short-term contact of selenite with pyrite and troilite indicate that these sulfide minerals react geochemically different.

■ 3602

Measurements of the Hygroscopic and Deliquescence Properties of Organic Compounds of Different Solubilities in Water and Their Relationship with Cloud Condensation Nuclei Activities

Man Nin Chan, Sonia M. Kreidenweis, and Chak K. Chan*

We study the hygroscopicity of atmospheric organic compounds of different water solubilities using an electrodynamic balance and discuss their relationship with cloud condensation nuclei activities.

■ 3609

Treatment of Dry Weather Urban Runoff in Tidal Saltwater Marshes: A Longitudinal Study of the Talbert Marsh in Southern California

Youngsul Jeong, Brett F. Sanders, Karen McLaughlin, and Stanley B. Grant*

Dry weather diversion of urban runoff improves the pollutant treatment capacity of a tidal saltwater marsh in southern California.

■ 3615

Organic Carbon—Water Concentration Quotients (II_{soc}s and \mathcal{T}_{poc} s): Measuring Apparent Chemical Disequilibria and Exploring the Impact of Black Carbon in Lake Michigan

Lawrence P. Burkhard*, Philip M. Cook, and Marta T. Lukasewycz

Corrections for black carbon partitioning yield plausible but inconclusive results.

3622

Improvement in Photocatalytic Activity of TiO₂ under Visible Irradiation through Addition of N-TiO₂

In-Cheol Kang*, Qiwu Zhang, Shu Yin, Tsugio Sato, and Fumio Saito

The mixing of anatase-TiO₂ and N-TiO₂ leads to higher photocatalytic activity under visible wavelength due to the effective depression of recombination rate between photoinduced electron and hole.

■ 3627

Lead Sequestration and Species Redistribution During Soil Organic Matter Decomposition

Andrew W. Schroth*, Benjamin C. Bostick, James M. Kaste, and Andrew J. Friedland

The speciation and sequestration of Pb in surficial organic rich soil horizons during decomposition varies over time and by forest type.

■ 3634

Enantioselective Bioaccumulation of Hexabromocyclododecane and Congener-Specific Accumulation of Brominated Diphenyl Ethers in an Eastern Canadian Arctic Marine Food Web

Gregg T. Tomy*, Kerri Pleskach, Tyler Oswald, Thor Halldorson, Paul A. Helm, Gordia MacInnis, and Chris H. Marvin

There is an enantioselective enrichment of the (–)α-enantiomer of hexabromocyclododecane in a food web from the eastern Canadian Arctic.

ENVIRONMENTAL MODELING

■ 3640

A GIS-based Approach for Modeling the Fate and Transport of Pollutants in Europe

A. Pistocchi

A screening-level pollutant fate and transport modeling approach is proposed, surrogating more complex models by exploiting map algebra and standard GIS techniques.

■ 3648

Geostatistical Modeling of the Spatial Distribution of Soil Dioxins in the Vicinity of an Incinerator. 1. Theory and Application to Midland, Michigan

Pierre Goovaerts*, Hoa T. Trinh, Avery Demond, Alfred Franzblau, David Garabrant, Brenda Gillespie, James Lepkowski, and Peter Adriaens

A geostatistical simulation-based methodology is described that combines the detailed process-based modeling of atmospheric deposition from an incinerator with the probabilistic modeling of residual field variability.

■ 3655

Geostatistical Modeling of the Spatial Distribution of Soil Dioxin in the Vicinity of an Incinerator. 2. Verification and Calibration Study

Pierre Goovaerts*, Hoa T. Trinh, Avery H. Demond, Timothy Towey, Shu-Chi Chang, Danielle Gwinn, Biling Hong, Alfred Franzblau, David Garabrant, Brenda W. Gillespie, James Lepkowski, and Peter Adriaens

Recently collected field data are used to assess the accuracy and precision and then update a geostatistical model of the spatial distribution of soil dioxin around an incinerator.

■ 3662

Statistical Modeling of Global Geogenic Fluoride Contamination in Groundwaters

Manouchehr Amini, Kim Mueller, Karim C. Abbaspour, Thomas Rosenberg, Majid Afyuni, Klaus N. Møller, Mamadou Sarr, and C. Annette Johnson*

Spatial distribution of groundwater fluoride concentrations is modeled on a global scale employing known geochemical processes and statistical procedures within the Geographic Information System environment.

■ 3669

▶ **Statistical Modeling of Global Geogenic Arsenic Contamination in Groundwater**

Manouchehr Amini, Karim C. Abbaspour, Michael Berg, Lenny Winkel, Stephan J. Hug, Eduard Hoehn, Hong Yang, and C. Annette Johnson*

Probability maps of groundwater arsenic contamination modeled on a global scale using statistical analysis based on measured arsenic data, physical variables, and known geochemical processes are presented.

■ 3676

Simulation of Air Quality Impacts from Prescribed Fires on an Urban Area

Yongtao Hu,* M. Talat Odman, Michael E. Chang, William Jackson, Sangil Lee, Eric S. Edgerton, Karsten Baumann, and Armistead G. Russell

Capabilities of an operational forecasting system to assess impacts of forest fires are studied and suggest significant emissions of isoprenoids increasing ozone and PM.

■ 3683

Sensitivity Analysis of Ozone Formation and Transport for a Central California Air Pollution Episode

Ling Jin, Shaheen Tonse, Daniel S. Cohan, Xiaoling Mao, Robert A. Harley, and Nancy J. Brown*

Spatial and temporal variations in ozone limiting reagents and local vs upwind source contributions are determined for an air pollution episode in Central California.

■ 3690

Dependence of Persistence and Long-Range Transport Potential on Gas-Particle Partitioning in Multimedia Models

Christian W. Götz, Martin Scheringer,* Matthew MacLeod, Fabio Wegmann, Urs Schenker, and Konrad Hungerbühler

When gas-particle partitioning is described with a poly-parameter linear free-energy model, increased long-range transport of polar semivolatile organic chemicals is observed.

■ 3697

Black Carbon-Inclusive Modeling Approaches for Estimating the Aquatic Fate of Dibenzo-*p*-dioxins and Dibenzofurans

James M. Armitage, Ian T. Cousins,* N. Johan Persson, Örjan Gustafsson, Gerard Cornelissen, Tuomo Saloranta, Dag Broman, and Kristoffer Næs

A black carbon-inclusive multimedia model for estimating the fate of dioxins and furans in a Norwegian fjord is developed and evaluated against field data.

■ 3704

Combining Long-Range Transport and Bioaccumulation Considerations to Identify Potential Arctic Contaminants

Gertje Czub,* Frank Wania, and Michael S. McLachlan

Mechanistic models link global emissions of hypothetical persistent chemicals to concentrations in Arctic Inuit.

■ 3710

Contribution of Volatile Precursor Substances to the Flux of Perfluorooctanoate to the Arctic

Urs Schenker, Martin Scheringer,* Matthew MacLeod, Jonathan W. Martin, Ian T. Cousins, and Konrad Hungerbühler

The global environmental fate of perfluorooctanoate and its precursor substances is simultaneously modeled; concentrations and fluxes compare well to atmospheric measurements and ice core data.

■ 3717

Assessing Contaminant Mobilization from Waste Materials: Application of Bayesian Parameter Estimation to Batch Extraction Tests at Varying Liquid-to-Solid Ratios

Sascha C. Iden,* Markus Delay, Fritz H. Frimmel, and Wolfgang Durner

Contaminant release from waste materials is studied using batch extraction tests to predict concentrations at liquid-to-solid ratios representative for in-situ conditions.

■ 3724

Fate of PBDEs in Juvenile Lake Trout Estimated Using a Dynamic Multichemical Fish Model

Satyendra P. Bhavsar,* Nilima Gandhi, Sarah B. Gewurtz, and Gregg T. Tomy

Biotransformation half-lives and gut absorption efficiencies of 13 major PBDE congeners in juvenile lake trout (*Salvelinus namaycush*) are estimated with a newly developed fugacity-based dynamic multichemical fish model.

ENVIRONMENTAL MEASUREMENTS METHODS

■ 3732

Evaluation of Statistical Treatments of Left-Censored Environmental Data using Coincident Uncensored Data Sets: I. Summary Statistics

Ronald C. Antweiler* and Howard E. Taylor

Nine common treatments of left-censored data for determination of summary statistics are evaluated.

3739

Extraction of Hexavalent Chromium from Chromated Copper Arsenate Treated Wood under Alkaline Conditions

Suzana Radivojevic and Paul A. Cooper*

Inconsistencies with respect to whether Cr(VI) is present in fixed CCA-treated wood are attributed to method-induced oxidation of Cr(III) in wood under alkaline extraction conditions.

■ 3745

Field Sampling Method for Quantifying Odorants in Humid Environments

Steven L. Trabue,* Kenwood D. Scoggin, Hong Li, Robert Burns, and Hongwei Xin

A field sampling and analysis method is developed for humid environments to quantify polar semivolatile compounds in air from animal feeding operations.

■ 3751

Perfluorinated Compounds in House Dust from Ohio and North Carolina, USA

Mark J. Strynar and Andrew B. Lindstrom*

Perfluoroalkyl acids (PFAAs) and fluorinated telomer alcohols (FTOHs) are measured in house dust samples collected from Ohio and North Carolina in 2000–2001.

■ 3757

Geophysical Monitoring of Hydrological and Biogeochemical Transformations Associated with Cr(VI) Bioremediation

Susan S. Hubbard,* Ken Williams, Mark E. Conrad, Boris Faybishenko, John Peterson, Jinsong Chen, Phil Long, and Terry Hazen

The utility of geophysical data sets for interpreting hydrobiogeochemical transformations associated with a remedial treatment in high resolution, over field relevant scales, and in a minimally invasive manner is illustrated.

■ 3766

Passive Sampling and Analyses of Common Dissolved Fixed Gases in Groundwater

Brian P. Spalding* and David B. Watson

Common fixed gases dissolved in groundwater can be collected passively in situ and directly analyzed by gas chromatography yielding total mixing ratios.

REMEDATION AND CONTROL TECHNOLOGIES

■ 3773

Secondary Effects of Catalytic Diesel Particulate Filters: Conversion of PAHs versus Formation of Nitro-PAHs

Norbert V. Heeb,* Peter Schmid, Martin Kohler, Erika Gujer, Markus Zennegg, Daniela Wenger, Adrian Wichser, Andrea Ulrich, Urs Gfeller, Peter Honegger, Kerstin Zeyer, Lukas Emmenegger, Jean-Luc Petermann, Jan Czerwinski, Thomas Mosimann, Markus Kasper, and Andreas Mayer

Effects of iron- and copper-catalyzed diesel particulate filters on emissions of aryl hydrocarbons, including genotoxic PAHs and nitro-PAHs, are investigated.

3780

Temperature Programmed Reduction for Measurement of Oxygen Content in Nanoscale Zero-Valent Iron

Jiasheng Cao, Xiaoqin Li, Javad Tavakoli, and Wei-xian Zhang*

Fresh nanoscale zero-valent iron is characterized with temperature programmed reduction and has average oxygen content at 8.21% and Fe(0) at 75.98%.

3786

Arsenate Removal by Nanostructured ZrO₂ Spheres

Kiril D. Hristovski,* Paul K. Westerhoff, John C. Crittenden, and Larry W. Olson

Highly porous nanostructured ZrO₂ spheres are synthesized and evaluated for adsorbent media in a packed bed adsorber using the pore surface diffusion model.

■ 3791

Fabrication of a TiO₂-BDD Heterojunction and its Application As a Photocatalyst for the Simultaneous Oxidation of an Azo Dye and Reduction of Cr(VI)

Hongbin Yu, Shuo Chen, Xie Quan,* Huimin Zhao, and Yaobin Zhang

An enhanced photocatalytic ability to oxidize azo dye and reduce Cr(VI) simultaneously is obtained by designing a heterojunction photocatalyst with TiO₂ and a boron-doped diamond.

■ 3797

Removal of Arsenic from High Ionic Strength Solutions: Effects of Ionic Strength, pH, and preformed versus in situ formed HFO

Kenneth L. Mercer* and John E. Tobiason

Experiments and modeling are conducted to assess arsenic removal by ferric iron addition to solutions with ionic strengths in the range of NF/RO membrane concentrates.

■ 3803

Dramatic Visible Photocatalytic Degradation Performances Due to Synergetic Effect of TiO₂ with PANI

Hao Zhang, Ruilong Zong, Jincal Zhao, and Yongfa Zhu*

Monolayer-dispersed PANI-modulated TiO₂ photocatalysts present synergetic effect to create remarkable visible photocatalytic performances as well as enhanced ultraviolet activities.

3808

Photocatalytic Degradation of Methanol Using Silica-Titania Composite Pellets: Effect of Pore Size on Mass Transfer and Reaction Kinetics

Jennifer M. Stokke* and David W. Mazyck

The efficiency of methanol degradation depends on the internal surface area of the composite and the space time of the gas in the reactor.

■ 3814

NO_x Removal from Simulated Flue Gas by Chemical Absorption—Biological Reduction Integrated Approach in a Biofilter

Shi-Han Zhang, Ling-Lin Cai, Xu-Hong Mi, Jin-Lin Jiang, and Wei Li*

The feasibility of NO_x removal by a chemical-biological integrated approach in a biofilter is experimentally investigated, and a mathematic model is developed to describe the process.

SUSTAINABILITY ENGINEERING AND GREEN CHEMISTRY

■ 3821

In Vitro Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal-Oxide Binding Archetype

Brian H. Lower,* Roberto D. Lins, Zachery Oestreicher, Tjerk P. Straatsma, Michael F. Hochella, Jr., Liang Shi, and Steven K. Lower

Peptide phage-display technology and molecular dynamics simulations are used to "unearth" a putative metal-oxide binding archetype that could be exploited to synthesize protein-metal-oxide nanostructures.

3828

Affinity of Microbial Fuel Cell Biofilm for the Anodic Potential

Ka Yu Cheng, Goen Ho, and Ralf Cord-Ruwisch*

The dependency of the microbial activity in a highly active microbial fuel cell on the potential of the electron-accepting electrode (anode) in a microbial fuel cell (MFC) is investigated.

■ 3835

Illuminating Tungsten's Life Cycle in the United States: 1975–2000

E. M. Harper* and T. E. Graedel

Inspired by recent attention focusing upon tungsten, a historical analysis in the United States indicates that most is initially imported, and a significant portion is eventually discarded.

■ 3843

Hybrid Input-Output Approach to Metal Production and Its Application to the Introduction of Lead-Free Solders

Shinichiro Nakamura,* Shinsuke Murakami, Kenichi Nakajima, and Tetsuya Nagasaka

A hybrid input-output model including the production process of non-ferrous metals was developed and applied to evaluating resource effects of lead-free solders.

3849

Approach for Energy Saving and Pollution Reducing by Fueling Diesel Engines with Emulsified Biosolution/Biodiesel/Diesel Blends

Yuan-Chung Lin, Wen-Jhy Lee, How-Ran Chao, Shu-Li Wang, Tsui-Chun Tsou, Guo-Ping Chang-Chien, and Perng-Jy Tsai*

Emulsification and biosolution additive provide useful approaches for saving energy and reducing emissions of particulate matters and polycyclic aromatic hydrocarbons from diesel-engine generators.

3856

► Arsenic in Rice: I. Estimating Normal Levels of Total Arsenic in Rice Grain

Yamily J. Zavala* and John M. Duxbury

Arsenic levels in rice from different U.S. states and other countries are compared and used to derive a global normal range.

■ 3861

► Arsenic in Rice: II. Arsenic Speciation in USA Grain and Implications for Human Health

Yamily J. Zavala,* Russell Gerads, Hakan Gürleyük, and John M. Duxbury

Speciation of arsenic in rice shows two broad types of rice, dominated by DMA (most U.S. rice) or inorganic As (most Asian and European rice).

3867

Total and Inorganic Arsenic Concentrations in Rice Sold in Spain, Effect of Cooking, and Risk Assessments

Silvia Torres-Escribano, Mariana Leal, Dinoraz Vélez,* and Rosa Montoro

The study reveals the need to consider the determination of inorganic As and the influence of cooking when evaluating the risks associated with the consumption of rice.

■ 3873

Comparative Population Analysis of Metallothionein Promoter Alleles Suggests Stress-induced Microevolution in the Field

Thierry K. S. Janssens, Ricardo del Rio Lopéz, Janine Mariën, Martijn J. T. N. Timmermans, K. Montagne-Wajer, Nico M. van Straalen, and Dick Roelofs*

Heavy metals in the environment exert selection on the metallothionein promoter of soil arthropods suggesting adaptation by altered transcriptional regulation.

■ 3879

Influence of Sediment-Amendment with Single-walled Carbon Nanotubes and Diesel Soot on Bioaccumulation of Hydrophobic Organic Contaminants by Benthic Invertebrates

P. Lee Ferguson,* G. Thomas Chandler, Ryan C. Templeton, Amanda DeMarco, Wally A. Scrivens, and Benjamin A. Englehart

Single-walled carbon nanotubes influence the bioaccumulation of sediment-associated hydrophobic organic contaminants by two estuarine deposit-feeding organisms.

■ 3886

A CL Mode Detector for Rapid Catalyst Selection and Environmental Detection Fabricated by Perovskite Nanoparticles

Fei Teng,* Tongguang Xu, Yang Teng, Shuhui Liang, Bulgen Gauge, Jie Lin, Wenqing Yao, Ruilong Zong, Yongfa Zhu,* and Youfei Zheng

A multiregion CL sensor for environmental combustible gases is investigated.

■ 3893

Bioaccumulation and Trophic Magnification of Short- and Medium-Chain Chlorinated Paraffins in Food Webs from Lake Ontario and Lake Michigan

Magali Houde, Derek C. G. Muir,* Gregg T. Tomy, D. Michael Whittle, Camilla Teixeira, and Serge Moore

Short- and medium-chain length chlorinated paraffins are widely distributed and undergo bioaccumulation in Lake Ontario and Lake Michigan food webs.

■ 3900

Comparison of Subcellular Partitioning, Distribution, and Internal Speciation of Cu between Cu-Tolerant and Naïve Populations of *Dendrodrilus rubidus* Savigny

Becky E. Arnold, Mark E. Hodson,* John Charnock, and Willie J. G. M. Peijnenburg

Despite exhibiting tolerance and accumulation of Cu, internal distribution, and speciation of Cu is the same in Coniston Copper mines and nearby naïve earthworm populations.

ADDITIONS AND CORRECTIONS

3906

Removal of *E. Coli* from Water Using Surface Modified Activated Carbon Filter Media and Its Performance over an Extended Use

Sukdeb Pal, J. Joardar, and Joon Myong Song*

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